



Towards a multi-scale analysis of dynamic failure in architected materials

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des matériaux des structures et des surfaces

Par

Elie EID

Towards a multi-scale analysis of dynamic failure in architected materials

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ABSTRACT

Architected materials are a rising class of materials that provide tremendous possibilities in terms of functional properties.

Interest is drawn on the failure of architected materials in which **scale separation ceases to exist**. This directly translates to strong interactions between a **crack tip** and the **architecture** independently of the considered scale. Moreover, under dynamic loadings, **stress-waves** come into play and **interactions** between the crack-tip, the microstructure (architecture) and the stress-waves eventually pilot together the structural behaviour.

In this thesis, three types of architected materials are considered: one **periodic** and two Penrose-type **quasi-periodic** lattices of holes. The analysis is broken into three parts.

To study the **influence of the microstructure on crack-propagation** at different scales, numerical simulations of failure are analysed; they show **improved resistance** to crack propagation in the quasi-periodic materials. At the core of the work is also the development of a coarse-graining technique that requires **no representative volume element**. This technique allows for a **physically consistent** multi-scale evaluation of the effective failure properties of the architectures. The inevitability of the consideration of a **non-homogeneous effective medium** to accurately model microstructural effects at larger scales is highlighted.

In dynamics, the influence of the architectures on the stress-wave attenuation shows **improved attenuation** properties of the quasi-periodic lattices.

Moreover, to understand the mechanism(s) governing the **dynamic branching** phenomenon in a homogeneous material, a criterion based on dynamic fracture mechanics is developed and validated on a novel experimental setup where **Ultra-High-Speed-High-Resolution imaging** is combined with **Digital Image Correlation** to capture extraordinary phenomena. The unquestionable role of **T-stress** in dynamic branching is put forth.

This thesis brings forth the necessary tools towards a multi-scale analysis of dynamic failure in architected materials.

Keywords: *Architected materials, coarse-graining, brittle fracture, dynamic fracture, crack branching*

RÉSUMÉ

Durant ces dernières années, on a vu un intérêt de plus en plus marqué pour de nouveaux matériaux avancés appelés **matériaux architecturés**.

On s'intéresse à la fissuration de matériaux architecturés dans lesquels la **séparation d'échelle n'est pas toujours bien établie**. Ceci se traduit par de fortes interactions entre le **front de la fissure** et l'**architecture** du matériau indépendamment de l'échelle considérée. De plus, sous chargements dynamiques, des ondes élastiques entrent en jeu et les **interactions** entre le front de la fissure, les ondes élastiques et la microstructure pilotent ensemble le comportement global de la structure.

Dans cette thèse, trois types de matériaux architecturés (microstructures) sont considérés : un réseau de trous **périodique** et deux réseaux **quasi-périodiques** type Penrose. L'analyse est divisée en trois parties.

Pour étudier l'influence de la microstructure sur la propagation des fissures à différentes échelles, des simulations numériques de rupture sont analysées ; ces simulations montrent une meilleure résistance des matériaux quasi-périodiques à la propagation des fissures. De plus, on développe une approche de changement d'échelle "bottom-up" qui n'a **pas recours à la notion de volume élémentaire représentatif**. Celle-ci permet donc une **évaluation multi-échelle cohérente** des propriétés effectives à la rupture des microstructures périodiques et quasi-périodiques. On montre ainsi l'inévitabilité de la prise en compte d'**un milieu effectif non-homogène** pour modéliser avec précision la réponse globale d'un matériau en tenant compte de sa sous-structure.

En dynamique, une analyse de l'influence de l'architecture **sur l'atténuation** des ondes élastiques montre une **meilleure performance** des réseaux quasi-périodiques.

De plus, pour comprendre le ou les mécanismes régissant le phénomène de **branchement dynamique** dans un milieu homogène, un critère basé sur la mécanique de la rupture dynamique est développé et validé sur une nouvelle configuration expérimentale où l'imagerie à **ultra haute vitesse et haute résolution** est combinée à la **corrélation d'images numériques** pour capturer les phénomènes marquants. Le rôle incontestable que joue la **contrainte T** dans le branchement dynamique est mis en avant.

Cette thèse fournit ainsi les outils nécessaires à une analyse multi-échelle

de la rupture dynamique des matériaux architecturés.

Mots-clés : *Matériaux architecturés, coarse-graining, rupture fragile, rupture dynamique, branchement*

À ma famille.

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GENERAL INTRODUCTION: BACKGROUND AND MOTIVATIONS

The desire for better-performing materials has long been established, and expansion of the boundaries of the material property space has already been achieved in multiple ways, i.e., whether by manipulating the chemistry, through developing new alloys and polymers, or by manipulating the microstructure through thermomechanical processing [Fleck et al., 2010]. Innovative materials for aerospace and automotive applications are recently requiring the improvement of the mechanical properties while reducing the structure's weight. Accordingly, engineers have shown interest in architected materials, i.e., in controlling the architecture of the materials through thoughtfully designing them in a certain fashion, to acquire improved mechanical properties over their constituents. With the developments in additive manufacturing techniques, demands on custom designed architectures to meet certain specifications have boomed, and with them research activities around this subject.

However, the real-life use of such highly heterogeneous materials is bridged by some limitations, in fact, despite the many powerful computational methods that have been developed in the last few decades, explicitly modelling the architectures for numerical simulations remains a heavy task. Thus, of course, it's practically appealing to describe a simpler nature of those materials to essentially assess their reliability and lifetime. So aside from determining their effective properties, there's a relevant need for incorporating small-scale mechanisms of deformation and damage in the analysis.

As scale-separation is not always well established in architected materials, classical homogenisation techniques fall short; plus, a weak scale-separation directly translates to strong interactions between fracture processes and the architecture independently of the considered scale. Accordingly, we believe that a consistent micro-meso analysis on the damage of highly heterogeneous materials' (architected materials between them) requires proceeding through multiple intermediate scales to ensure proper modelling between the scales.

Besides, Quasi-Periodic architected materials have attracted increasing attention

among the scientific community due to their extraordinary acoustic and elastic wave propagation performances. These microstructures are shown to exhibit complex vibrational behaviour, including a set of frequency ranges in which no propagative wave exists, i.e., band gaps. Based on their wavelengths, the stress-waves' behaviour inside architected materials would vary.

Now imagine a crack immersed in such architectures under dynamic loading; the crack tip would 'see' a continuous variation of the stress state at its vicinity coming from the back-and-forth reflections of the stress-waves at the free boundaries of the architecture. Even in homogenous materials, the problem is complex, since stress-waves reflected from the boundaries and others emitted by the crack tip will alternatively load and unload the crack tip. Evidently, the interactions between the crack-tip, the microstructure (architecture) and the stress-waves eventually pilot together the structural behaviour. Accordingly, we believe that transient analysis should always be considered. Further, we believe that understanding the interaction between stress-waves and crack tips, debuting with homogenous materials, should build the foundation for future analysis of the dynamic fracture of architected materials, i.e., where a range of mixed and complex stress-waves reflections and interactions with the crack tip are expected.

So what's the plan?

We aim at analysing the interaction between the microstructure from one side (material), the stress-wave and crack propagation (loading) from the other, the analysis is followed on one Periodic and two Penrose-type-Quasi-Periodic architectures. Eventually, the purpose of the present PhD work is to provide contributions to the above-mentioned challenges and advance the necessary tools towards a multi-scale analysis of dynamic failure of the architected materials.

We first propose a versatile model-free coarse-graining approach (adapted from [Goldhirsch and Goldenberg, 2002]'s work in Molecular Dynamics) that is indeed applicable on cases where the statistical homogeneity of the material ceases to exist (Quasi-Periodic materials with long-range heterogeneities) and more importantly when sharp localisations are present.

The problem is then broken down into three sub-problems -as shown in Figure 1- and we devote one chapter for each.

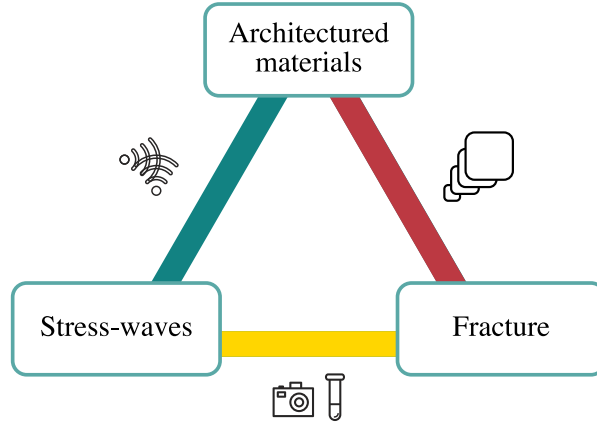


Figure 1 – The holy trinity of this PhD

On the crack propagation in architected materials (Chapter 3), the following questions are asked:

- ▶ How does the architecture influence a propagating crack?
- ▶ How to assess the effective failure properties and what determines them (microscopically)?
- ▶ How are the effective failure properties linked to the length-scales?
- ▶ To what extent can an effective homogeneous model accurately replace the microstructural behaviour?

On the stress-wave propagation inside the architected materials (Chapter 4), the following questions are addressed:

- ▶ How does the stress-waves' wavelengths influence their propagation inside the architected materials?
- ▶ How does the architectures damp the stress-waves' energy?
- ▶ How are the stress-waves modified as they propagate inside architected materials?

On the stress-waves and their role in crack propagation (Chapter 5), the following questions are addressed:

- ▶ How do stress-waves affect crack propagation?
- ▶ Why do cracks branch? and at what crack tip speeds?
- ▶ How to explain the limiting velocities observed in the experiments?
- ▶ How to explain the limiting velocities observed in the numerical phase-field simulations?
- ▶ Why do damage bands sometimes thicken in phase-field models?

Outline of the PhD thesis

The preliminary Chapter 0 presents a concise literature review of the theoretical concepts relevant to brittle fracture, architected materials, numerical simulations and homogenisation techniques. The goal of this chapter is of course to provide the reader with the concepts at the base of the present work.

After contextualising and motivating the problem and providing the necessary theoretical background, Part II concerns the computational approach considered in this work. The numerical simulation of failure, based on the phase-field approach to fracture (see e.g., [Miehe et al., 2010a]), is broadly brought forth and discussed in Chapter 1. After presenting the phase-field model, an extension is proposed by parametrising the elastic strain threshold (for the quadratic crack density function), and linking it to other phase-field parameters. Application and validation of the influence of this parametrisation on the material response are lead on two benchmarks, one quasi-static and another dynamic.

Chapter 2 provides the detailed development of the coarse-graining method adapted from [Goldhirsch and Goldenberg, 2002]. At the end of this chapter, the proposed method is validated and compared to classical upscaling (homogenisation) techniques. The method is shown to accurately predict the effective elasticity tensor, but more prominently it gives insights on the effective behaviour of the material at different intermediate scales. The applicability of the method in cases where sharp localisation exist is indeed validated, and a bridge between fracture mechanics and damage mechanics is built.

After advancing the computational methods in Part II, the first pillar of this thesis is tackled: the interaction between a propagating crack and microstructures (architectures) (Part III, Chapter 3). The proposed scheme relies on simulating the failure process of architected materials at the microscopic scale via the Phase field model (from Chapter 1). The acquired information is then upscaled to mesoscopic scale(s) by the means of the proposed model-free coarse-graining technique.

The two dynamics thematics are then tackled: the propagation of stress-waves inside architected materials and the dynamic propagation of cracks.

Chapter 4 covers the interactions between stress-waves and the microstructure by applying sinusoidal waves of different wavelengths at one boundary and analysing the output stress waves from the opposite. Finite element simulations of transient wave propagation are considered for this purpose, and analysis on the energy damping and stress-wave scattering is lead.

Chapter 5 wraps up this thesis by analysing the role played by stress-waves in crack propagation in homogeneous materials. Unlike in previous chapters, where the numerical simulations of damage are at the core of the developments, this chapter is based on simple dynamic fracture mechanics concepts applied on a novel experimental setup. By exploiting Ultra-High-Speed-High-Resolution (UHS-HR) imaging and cutting edge digital image correlation *DIC* algorithms, a novel inertial impact experimental configuration would shed light on the phenomena of branching at limiting velocities. Moreover, the application of the analysis scheme on a phase-field crack branching benchmark would yield more comprehension on this phenomenon.

PART I

Literature review

LITERATURE REVIEW

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0.1 Introduction

As a preliminary, this first chapter aims to present a concise literature review. General concepts relevant to **fracture mechanics**, **architected materials**, **numerical simulations** of brittle fracture and **homogenisation techniques** are put forth. The goal is to prepare the ground for the upcoming developments and advancements in the following chapters.

First, generalities regarding linear elastic fracture mechanics are showcased: the asymptotic solutions of the stress and displacement fields are given. Then the asymptotic fields near a moving crack-tip are described. Crack initiation and propagation criteria are only exposed briefly, as more details are to be given in Chapter 5, when tackling the dynamic branching problem.

Second, the available numerical methods for modelling crack propagation in brittle materials are reviewed and the advantages of considering the phase-field model for this thesis are stressed.

Third, a historical perspective regarding the expansion of the material property space with the expanding desire for better-performing materials is given. Focus is shed on the architected materials. The Periodic and Quasi-Periodic microstructures in question in this work are presented.

We finish covering every topic related to this thesis by overviewing the classical homogenisation techniques and their underlying limitations regarding the requirement of separation of scales, and dealing with sharp localisations (crack, high heterogeneities) between others. Moreover, recent advancement in the field of homogenisation of a damage model are presented. Finally, the *bottom-up* approach that will be exploited to accurately portray the failure of architected materials at larger scales is introduced.

Remark 0.1. *The computational methods directly related to this work are detailed in the next Part. Analysis and investigation on the phase-field model will be presented in Chapter 1, by the end of which an extension to the framework is proposed. The coarse-graining technique is derived in Chapter 2, and numerically validated on simple examples.*

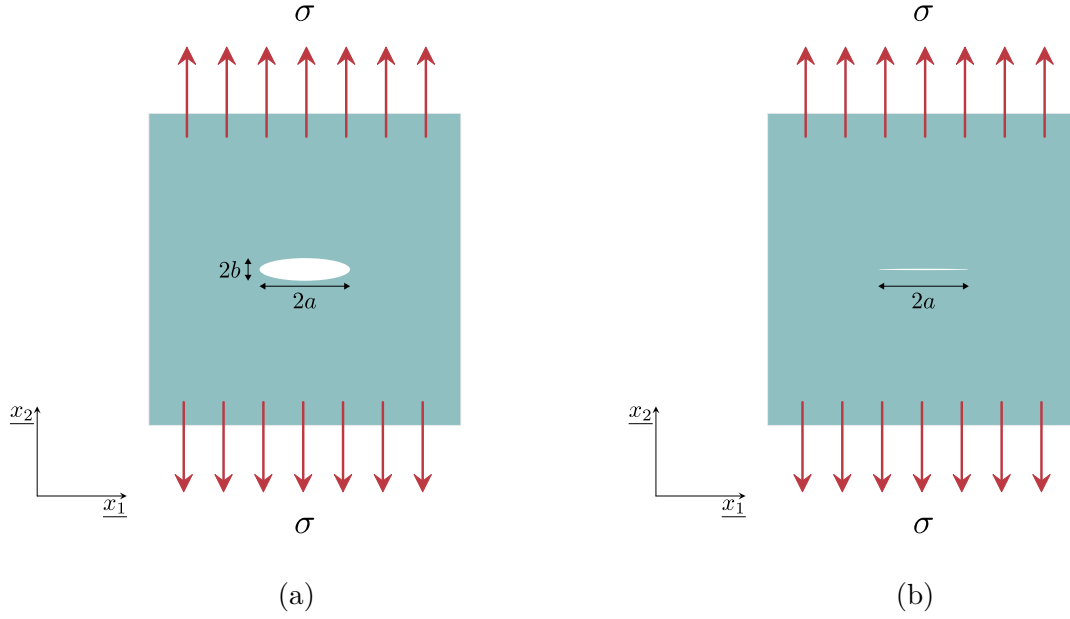


Figure 2 – Infinite plate subjected to uniform applied tension with defects: an elliptical defect of semi-axes a and b (a), a slit crack of length $2a$ (b)

0.2 Dynamic fracture mechanics

0.2.1 Linear Elastic Fracture Mechanics (LEFM)

Based on an energetic approach from the twentieth century, LEFM is a robust theoretical framework to predicting crack propagation in homogeneous media. We briefly summarize the main milestones of the fracture mechanics developments along with its fundamental elements. These elements would constitute the core of Chapter 5, but of course, a starting point for the numerical methods for crack propagation (Chapter 1) and their application in Chapter 3.

Basic concepts

[Inglis, 1913] was the first to study the distribution of stress in an infinite plate containing a defect: an elliptical hole of semi-axes a in the x -direction and b in the y -direction (Figure 2).

He showed that under a uniform applied tension σ , the opening stress at the defect σ_O

is amplified by a certain geometrical factor related to the defect geometry:

$$\sigma_O = (1 + 2\frac{a}{b})\sigma \quad (1)$$

When the defect becomes sharp, ($b \ll a$), the local stresses become singular. The theory of linear elastic fracture mechanics studied this stress singularity and aimed at characterising the stress-field near the crack front.

Near-tip asymptotic solution

The stress-field around a crack-tip in a linear elastic isotropic material was first established by [Westergaard, 1939] and is based on the Airy stress function concept. The solution is only valid when non-linear and inelastic deformations are small or are confined in a small zone near the crack-tip compared to the size of the crack. From the near-crack-tip approximation of the [Westergaard, 1939] solution of the stress-field surrounding the crack, [Irwin, 1957] defined the so-called 'stress intensity factors' *SIF*. The near-tip associated stresses were re-written in terms of those stress intensity factors and an inverse square root singularity was found at the crack-tip. For a semi-infinite straight crack in a 2D elastic body -of shear modulus μ and Poisson ratio ν - subjected to a mechanical load, [Williams, 1957] proposes higher order analytical solutions of symmetric (opening mode *I*) and antisymmetric (in-plane shear mode *II*) fracture modes. These modes of fracture would eventually depend on the loading conditions and the geometry of the body. A typical sketch of the modes is presented in Figure 3, showing the opening and sliding of modes *I* and *II* [Rice, 1968]; the out-of-plane mode *III* shearing (tearing) is disregarded in our study.

Here, the leading terms of the in-plane displacement field $\underline{u}$ at the vicinity of the crack-tip in Cartesian coordinates are given in terms of the *SIF* as follows:

$$\begin{aligned} u_1(r, \theta) &= \frac{K_I}{2\mu} \sqrt{\frac{r}{2\pi}} (\kappa - \cos \theta) \cos \frac{\theta}{2} + \frac{K_{II}}{2\mu} \sqrt{\frac{r}{2\pi}} (\kappa + \cos \theta + 2) \sin \frac{\theta}{2} \\ u_2(r, \theta) &= \frac{K_I}{2\mu} \sqrt{\frac{r}{2\pi}} (\kappa - \cos \theta) \sin \frac{\theta}{2} - \frac{K_{II}}{2\mu} \sqrt{\frac{r}{2\pi}} (\kappa + \cos \theta - 2) \cos \frac{\theta}{2} \end{aligned} \quad (2)$$

where K_I and K_{II} represent the mode *I* opening and mode *II* plane shear loading respectively, r and θ are the polar coordinates with respect to the crack-tip (Figure 4). κ is the Kolossov's constant that takes the value $\kappa = (3 - 4\nu)$ for plane strain conditions and $\kappa = (3 - \nu)/(1 + \nu)$ for plane stress. The expression of the in-plane stresses as a function

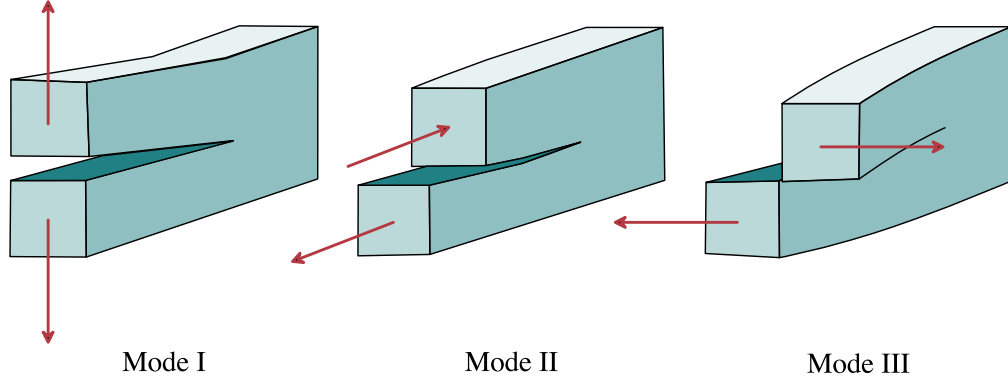


Figure 3 – Three modes of fracture: opening (mode *I*), in-plane shear (mode *II*) and out-of-plane shear (mode *III*), in this study, only the in-plane modes *I* & *II* are considered

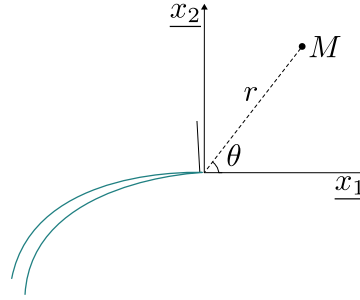


Figure 4 – The local polar coordinates around a crack-tip

of the leading terms reads:

$$\begin{aligned}
 \sigma_{11} &= \frac{K_I}{2\pi r} \left(1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \cos \frac{\theta}{2} - \frac{K_{II}}{2\pi r} \left(1 + \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \right) \sin \frac{\theta}{2} \\
 \sigma_{12} &= \frac{K_I}{2\pi r} \cos \frac{\theta}{2} \sin \frac{\theta}{2} \cos \frac{3\theta}{2} + \frac{K_{II}}{2\pi r} \left(1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \cos \frac{\theta}{2} \\
 \sigma_{22} &= \frac{K_I}{2\pi r} \left(1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \cos \frac{\theta}{2} + \frac{K_{II}}{2\pi r} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cos \frac{3\theta}{2}
 \end{aligned} \tag{3}$$

The next terms in the expansion involve the so-called *T – stress* for mode *I* and the rigid body rotation for mode *II*; those represent the non-singular uniform terms present in [Williams, 1957]’ expansion. For a semi-infinite crack propagating along the 11 direction under mixed loading, with the addition of the *T – stress*, the crack-parallel stress component

becomes:

$$\sigma_{11} = \frac{K_I}{2\pi r} \left(1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \cos \frac{\theta}{2} - \frac{K_{II}}{2\pi r} \left(1 + \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \right) \sin \frac{\theta}{2} + \mathbf{T} \quad (4)$$

Besides, it's mentioned that LEFM is found around the notion of small-scale yielding. This assumes that the processes leading to fracture i.e., coalescence of micro-defects, mechanisms of deformation, etc., actually happen in a confined zone called fracture process zone much smaller than the structure. The small scale yielding incorporates the notion that, even if in the confined vicinity the material no longer exhibits linear elastic behaviour, the leading *SIF* terms still govern the deformation state within.

Propagation criterion under mode *I* loading

Of course, the previous quantitative description of the stress state enables the use of phenomenological criteria to describe the conditions under which a crack can propagate. Knowing that the stresses are singular at the crack-tip, a propagation criterion based on a critical opening stress would be irrelevant. [Irwin, 1958] proposed a propagation criterion in mode *I* based on its associated *SIF* by defining an associated critical *SIF*_{*c*} (*K*_{*IC*} for mode *I*). The criterion can be summarized as follows:

$$\begin{aligned} K_I < K_{IC} &\leftarrow \text{crack does not propagate,} \\ K_I &= K_{IC} \leftarrow \text{stable crack propagation,} \\ K_I > K_{IC} &\leftarrow \text{unstable crack propagation.} \end{aligned} \quad (5)$$

It's noted that the crack extension mode *I* *SIF* *K*_{*I*}, is associated with a corresponding strain energy release rate, *G*_{*I*} via:

$$G = \frac{K_I^2}{E'} \quad (6)$$

where *E*' = *E* in plane stress and *E*' = $\frac{E}{1-\nu^2}$ in plane strain assumption. *E* here corresponds to Young's modulus of the bulk.

This yields the Griffith-Irwin [Irwin, 1958, Sanders Jr, 1960] fracture theory stating that a crack propagates when the stress intensity factor reaches a critical value *K*_{*IC*} (Equation 5), equivalently, when the energy release rate overcomes a critical value *G*_{*C*} (Equation 6).

Remark 0.2. A similar *SIF* criterion was derived under pure mode *II* where *K*_{*II*} is compared to its critical counterpart *K*_{*IIc*}, and to it is associated an energy release rate *G*_{*II*} = $\frac{K_{II}^2}{E'}$ compared to a critical value *G*_{*IIc*}.

Propagation criterion under mixed-mode loading

Any loading state is a combination of three independent stress intensity factors, as stated by [Irwin, 1957], hence the necessity to define a mixed-mode propagation criterion that can predict when a crack would propagate and along which direction. In this work, this feature (ability to predict fracture direction) would require the to-be-considered criterion to be readily and easily extended to dynamics as it will constitute the core of the developments related to Chapter 5. In the literature, a multitude of criteria were proposed [Cotterell and Rice, 1980, Erdogan and Sih, 1963, Hussain et al., 1974, Gupta, 1976, Palaniswamy and Knauss, 1978, Williams and Ewing, 1972], that are usually based on either energy or maximum circumferential-stress criteria. The maximum circumferential stress $\sigma_{\theta\theta}$ criterion first proposed by [Erdogan and Sih, 1963]) is considered. This criterion determines the direction of the maximum tensile stress, from one side, and can be used to compare the stress states and hence predict crack propagation condition from another. Details about the $\sigma_{\theta\theta}$ criterion are given directly in dynamics in Chapter 5, prior to the developments.

0.2.2 Extension to asymptotic fields near a moving crack-tip

Dynamic stress intensity factors

Multiple efforts were drawn on the determination of the dynamic counterpart of LEFM. [Broberg, 1960], [Baker, 1962] and others developed relations for the dynamic stress intensity factor, and they related the dynamic *SIF* (K_{kD}) to their static counterparts through universal functions k_k of the instantaneous crack-tip velocity v_c as follows:

$$K_{kD}(t) \simeq k_k(v_c)K_k(t) \quad (7)$$

The universal functions -that depend solely on the material parameters through the stress wave speed- are slightly different in the different solutions, here the following expressions are considered:

$$\begin{aligned} k_I(v_c) &= S\left(-\frac{1}{v_c}\right) \frac{1 - v_c/c_R}{\sqrt{1 - v_c/c_d}} \\ k_{II}(v_c) &= S\left(-\frac{1}{v_c}\right) \frac{1 - v_c/c_R}{\sqrt{1 - v_c/c_s}} \end{aligned} \quad (8)$$

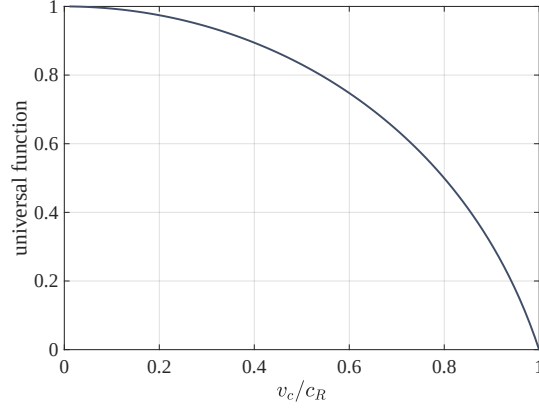


Figure 5 – The universal function $k_I(v_c)$ versus the normalised crack-tip speed (v_c/c_R)

where $S(\zeta)$ is given by:

$$S(\zeta) = \exp \left[-\frac{1}{\pi} \int_{1/c_d}^{1/c_s} \tan^{-1} \left(\frac{(4\eta^2 \sqrt{(\eta^2 - c_d^{-2})(c_s^{-2} - \eta^2)})}{(c_s^{-2} - 2\eta^2)^2} \right) \times \frac{d\eta}{\zeta + \eta} \right] \quad (9)$$

Here, c_R , c_d and c_s are Rayleigh, dilatational and shear wave speeds respectively. It's apparent that for each fracture mode, in the static configuration ($v_c/c_R = 0$ and $k_I = k_{II} = 1$), the unicity of the *SIF* are recovered $K_k = K_{kD}$. Figure 5 shows the dimensionless universal function k_I herein considered versus the normalised crack-tip speed v_c/c_R in plane strain assumptions.

Asymptotic fields in dynamics

[Freund and Hutchinson, 1992] gave an expression of the stress and displacement fields around a moving crack-tip that are function of the *SIF* (the leading terms only) and the crack-tip speed.

The displacements are given by:

$$u_i = \sum_{k=I,II} K_{kD} \sqrt{\frac{2}{\pi}} U_i^k(\theta, v_c) \quad (10)$$

For mode I opening:

$$\begin{aligned} U_1^I(\theta, v_c) &= \frac{1}{\mu D(v_c)} \left[(1 + \beta_s^2) \sqrt{r_d} \cos \frac{\theta_d}{2} - 2\beta_s \beta_d \sqrt{r_s} \cos \frac{\theta_s}{2} \right] \\ U_2^I(\theta, v_c) &= -\beta_d(1 + \beta_s^2) \sqrt{r_d} \sin \frac{\theta_d}{2} + 2\beta_d \sqrt{r_s} \sin \frac{\theta_s}{2} \end{aligned} \quad (11)$$

For mode II plane shear loading:

$$\begin{aligned} U_1^{II}(\theta, v_c) &= \frac{1}{\mu D(v_c)} \left[2\beta_s^2 \sqrt{r_d} \sin \frac{\theta_d}{2} - \beta_s(\beta_s^2 + 1) \sqrt{r_s} \sin \frac{\theta_s}{2} \right] \\ U_2^{II}(\theta, v_c) &= \frac{1}{\mu D(v_c)} \left[2\beta_s \beta_d \sqrt{r_d} \sin \frac{\theta_d}{2} - (\beta_s^2 + 1) \sqrt{r_s} \cos \frac{\theta_s}{2} \right] \end{aligned} \quad (12)$$

The stresses are given by:

$$\sigma_{ij} = \sum_{k=I,II} \frac{K_{kD}}{\sqrt{2\pi}} S_{ij}^k(\theta, v_c) \quad (13)$$

For mode I opening:

$$\begin{aligned} S_{11}^I(\theta, v_c) &= \frac{1}{D(v_c)} \left[(1 + \beta_s^2)(1 + 2\beta_d^2 - \beta_s^2) \frac{\cos \frac{\theta_d}{2}}{\sqrt{r_d}} - 4\beta_s \beta_d \frac{\cos \frac{\theta_s}{2}}{\sqrt{r_s}} \right] \\ S_{12}^I(\theta, v_c) &= \frac{2\beta_d(1 + \beta_s^2)}{D(v_c)} \left[\frac{\sin \frac{\theta_d}{2}}{\sqrt{r_d}} - \frac{\sin \frac{\theta_s}{2}}{\sqrt{r_s}} \right] \\ S_{22}^I(\theta, v_c) &= -\frac{1}{D(v_c)} \left[(1 + \beta_s^2)^2 \frac{\cos \frac{\theta_d}{2}}{\sqrt{r_d}} - 4\beta_s \beta_d \frac{\cos \frac{\theta_s}{2}}{\sqrt{r_s}} \right] \end{aligned} \quad (14)$$

and for mode II plane shear loading:

$$\begin{aligned} S_{11}^{II}(\theta, v_c) &= -\frac{2\beta_s}{D(v_c)} \left[(1 + 2\beta_d^2 - \beta_s^2) \frac{\sin \frac{\theta_d}{2}}{\sqrt{r_d}} - (1 + \beta_s^2) \frac{\sin \frac{\theta_s}{2}}{\sqrt{r_s}} \right] \\ S_{12}^{II}(\theta, v_c) &= \frac{1}{D(v_c)} \left[4\beta_s \beta_d \frac{\cos \frac{\theta_d}{2}}{\sqrt{r_d}} - (1 + \beta_s^2) \frac{\cos \frac{\theta_s}{2}}{\sqrt{r_s}} \right] \\ S_{22}^{II}(\theta, v_c) &= \frac{2\beta_s(1 + \beta_d^2)}{D(v_c)} \left[\frac{\sin \frac{\theta_d}{2}}{\sqrt{r_d}} - \frac{\sin \frac{\theta_s}{2}}{\sqrt{r_s}} \right] \end{aligned} \quad (15)$$

with

$$\begin{aligned}
D(v_c) &= -4\beta_s\beta_d - (1 + \beta_s^2)^2 \\
\beta_d &= \sqrt{1 - \left(\frac{v_c}{c_d}\right)^2} \\
\beta_s &= \sqrt{1 - \left(\frac{v_c}{c_s}\right)^2}
\end{aligned} \tag{16}$$

and

$$\begin{aligned}
(r_d, \theta_d) & / r_d e^{i\theta_d} = x_1 + i\beta_d x_2 \\
(r_s, \theta_s) & / r_s e^{i\theta_s} = x_1 + i\beta_s x_2
\end{aligned} \tag{17}$$

Of course, only the leading terms of the stress-field are considered and the non-singular uniform term, i.e., T – stress could be added to the expression of the stresses parallel to the crack path.

For a semi-infinite crack propagating along the 11 direction at crack-tip speed v_c under mixed loading, the stress at location (r, θ) under mixed loading becomes:

$$\sigma_{11} = \sum_{k=I,II} \frac{K_{kD}}{\sqrt{2\pi}} S_{11}^k(\theta, v_c) + \mathbf{T} \tag{18}$$

The main contrast with the quasi-static case is the dependence of the dynamic asymptotic fields on the crack-tip speed v_c , making any crack propagation criterion more difficult to perceive [Yoffe, 1951, Freund and Hutchinson, 1992].

Details about this modification of the stress distribution around a crack-tip (propagating at speed v_c) via the maximum circumferential stress criterion will be given in Chapter 5 as a simple yet efficient tool for analysing (in)stabilities of fast running cracks in homogeneous materials under rapidly varying loadings.

0.3 Numerical crack propagation simulation

As this study mainly focuses on the response of architected materials (highly heterogeneous materials, see Section 0.4) to crack propagation, a robust and versatile numerical method is required.

The theoretical methods to model brittle fracture [Griffith, 1921, Freund and Hutchinson, 1992] permitted the development of criteria for crack propagation in simple configura-

tions (homogeneous bodies, propagation of a single existing crack, etc.). However, such approaches fail to describe crack initiation or more complex phenomena like coalescence and branching. Many numerical simulation methods for crack propagation have been developed in the recent decades, and this section gives a quick overview of the most relatively popular methods: classical damage models, cohesive zone models, the thick level set method and the phase-field approach to fracture.

0.3.1 Damage models

The development of damage mechanics began in 1958 with [KACHANOV, 1958]. Beforehand, macroscopic failure criteria based only on fracture mechanics were proposed. As opposed to fracture mechanics, damage mechanics interest in a progressive deterioration of the material preceding its fracture [Lemaître and Chaboche, 1990].

§ 0.1. *On the differentiation between damage and fracture*

Physically speaking, the difference between fracture and damage are recalled as:

- **Damage:** Discontinuities on the smaller scales of the material (micro-cracks, micro-voids) that translate to a loss in rigidity of the 'macroscopic' sample. It's an irreversible process.
- **Fracture:** Discontinuities on the 'macroscopic' scale, leading to a global failure of the sample. So of course, from these definitions, one may guess that the former is at the source of the latter.

[KACHANOV, 1958] published the first paper devoted to a continuous **damage** variable, by writing a softening constitutive law:

$$\underline{\underline{\sigma}} = (1 - D)\mathbb{C}\underline{\underline{\varepsilon}}, \quad (19)$$

σ and ε are the Cauchy stress and strain tensors, respectively and $\mathbb{C}$ is the sound elastic tensor. D is an isotropic damage variable that takes the value of 1 corresponding to a breaking of the material, 0 in the sound material and $0 \leq D \leq 1$ to represent the deterioration of the material. Within the finite element FE context, softening behaviour is found to cause spurious mesh sensitivity and incorrect convergence when the element is refined to zero. Cohesive crack models [Xu and Needleman, 1994], crack band models [Baian and Cedolin, 1983] and regularised models were considered to overcome these limitations. Regularised models are based on the general continuum theory where internal

length and/or higher-order strain gradients are introduced. The focus will be drawn on the non-local damage theory. The work of [Bažant and Jirásek, 2002] introduces an internal length into the softening behaviour law; where local internal variables are replaced by their non-local counterparts, i.e., their spatial average. The size of the non-local zone is considered as a characteristic of the material:

$$\underline{\underline{\sigma}} = (1 - D)\mathbb{C}\underline{\underline{\tilde{\varepsilon}}}, \quad (20)$$

where $\underline{\underline{\tilde{\varepsilon}}}$ can be any non-local equivalent estimation of the strain tensor ε . Despite their ability to remedy the issues encountered in the FE implementations, these methods have the following drawbacks [Pijaudier-Cabot and Bažant, 1987]:

- ✗ **Incorrect prediction of damage initiation**
- ✗ **Deficiency in simulating branching**
- ✗ **Diffusion of damage zones even after complete failure**

More in-depth information about these models can be found in [Pijaudier-Cabot and Bažant, 1987, Bažant and Jirásek, 2002]..

0.3.2 Cohesive zone models

Because of its versatility, the cohesive zone model is being increasingly used to simulate discrete fracture processes in a number of homogeneous and inhomogeneous materials [Zhou and Molinari, 2004, Xu and Needleman, 1994, Dugdale, 1960]. The model typically relies on a separation of the crack surfaces - a phenomenon that is considered to take place across the extension of the physical crack-tip (in a cohesive zone), resisted by cohesive tractions. The cohesive law defines the constitutive relation between the surface traction and the relative opening displacement at the crack-tip. However, by constraining the crack propagation along the element edges, this approach suffers from mesh dependency. An overview of cohesive elements techniques can be found in [Chandra et al., 2002].

0.3.3 Thick level set

More recently, a Thick Level-Set (TLS) [Moës et al., 2011] damage approach was developed. Here, the fully degraded material is embedded at the core of a partially damaged zone of size l_c . A level-set Λ is used to separate the undamaged zone from the damaged zone, it's perceived as a signed distance function. A schematic representation

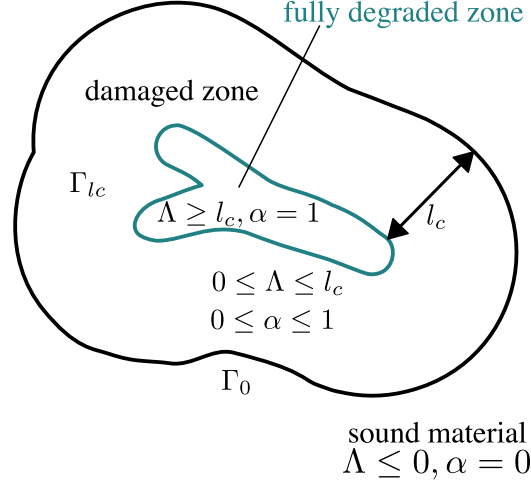


Figure 6 – Thick level set: damage α and level set Λ distribution

from [Moës et al., 2011] is displayed in Figure 6. The damage variable and its evolution are an explicit function of the level set. This function is a parameter of the model. The damage increases progressively as the level set value rises following inequalities (Figure 6):

$$\begin{aligned} \alpha(\Lambda) &= 0, & \text{if } \Lambda \leq 0 \\ \alpha(\Lambda) &\geq 0, & \text{if } 0 \leq \Lambda \leq l_c \\ \alpha(\Lambda) &= 1, & \text{if } \Lambda \geq l_c \end{aligned} \tag{21}$$

This method is able to describe complex crack phenomena like branching. Since damage evolution is dealt with via a level set function, the level set may be solved close only to the damaged zone which boosts the computational efficiency.

0.3.4 Phase-field approach to fracture

With the expected complex crack networks in our present work, techniques like X-FEM [Moes et al., 1999] that require the predefinition of a crack and/or cohesive element methods [Xu and Needleman, 1994] that only allow separations on mesh's boundary are discarded. The variational approach [Francfort, 1998] known as phase-field method is considered for building the micro-mechanical numerical experiments. The robustness and versatility of the approach regarding its independence of the FE discretisation were decisive

in the choice of the phase-field model for the micro-mechanical simulations. The phase-field method is based on a diffuse representation of the localised discontinuity coming from the presence of a crack. A regularized variational principle describes the evolution of the mechanical problem from one side, and the evolution of an additional damage field α describing the damage state from the other. The typical Griffith's-type problems are rewritten in a variational framework [Francfort, 1998, Bourdin et al., 2008] leading to an energy functional resembling the potential presented by [Mumford and Shah, 1989]. The various advantages of using the phase-field over other methods are summarised as follows:

- ✓ **One criterion to rule them all:** since phase-field modelling is purely based on energy minimisation, **no** artificial criteria for crack initiation, crack coalescence or crack branching should be added
- ✓ **Adaptability to multi-physics:** thanks to its variational structure, phase-field modelling allows to naturally incorporate multi-field physics problems.
- ✓ **Straightforward adaptation in 2D and 3D:** without sensitivity to mesh (respecting the convergence conditions)
- ✓ **Γ – convergence to [Griffith, 1921] theory:** theoretical proofs exist for the original theory. [Linse et al., 2017, Bellettini and Coscia, 1994, Chambolle, 2004]

Despite the major advantages of using phase-field modelling, the method suffers from the following drawbacks:

- ✗ **High computational cost:** to accurately resolve the gradient term, sufficiently refined mesh in the expected damage zone is crucial for the simulations
- ✗ **Inaccurate location of the crack-tips:** just like other continuous approaches, the phase-field modelling does not explicitly represent the crack (discontinuity). Arbitrary choices have to be taken, e.g., iso-curves of the phase-field [Borden et al., 2012], to predict the crack-tip. This leads to slightly inaccurate predictions of the crack velocity for dynamic fracture.

Despite the presented drawbacks, the relative ease of implementation of the phase-field model, the ease with which the method handles complex crack networks and extraordinary phenomena (growth, branching, merging), and the rigorous variational structure, are decisive in the choice of the phase-field model in this work. The computational framework as proposed by [Miehe et al., 2010b] is applied and an extension (parametrisation of the elastic threshold) to the original formulation is suggested (in Section 1.8). Original applications regarding static and dynamic simulation of fracture are tackled.

After familiarising the reader with the relevant notions regarding crack propagation, the next section focuses on presenting the architected materials that will be investigated in this study.

0.4 Architected materials

The desire for better-performing materials has long been established, and expansion of the boundaries of the material property space has already been achieved in multiple ways, i.e., whether by manipulating the chemistry, through developing new alloys and polymers, or by manipulating the microstructure through thermomechanical processing [Fleck et al., 2010]. Innovative materials for aerospace and automotive applications are recently requiring the improvement of the mechanical properties while reducing the structure's weight.

0.4.1 A new class of materials

Accordingly, engineers have shown interest in controlling the architecture of the materials through thoughtfully designing them in a certain fashion, to acquire improved mechanical properties over their constituents.

The ability of architected materials to give a wide range of stiffness, strength and fracture toughness is provided by the properties of the bulk material and the interplay between the shape, the periodicity, and the possible association of materials [Bouaziz et al., 2008].

A general architected material is made up of a large number of uniform elements (e.g., holes, inclusions, beams, rods, etc) and is generated by tessellating these elements on specific plane shapes (e.g., hexagonal, square, kites, darts, etc.) throughout space [Fleck et al., 2010].

One of the goals of this work is to assess the multi-scale behaviour of such materials regarding crack propagation. Periodic and Quasi-Periodic microstructures are considered in the study, with the idea that any material would behave between a perfectly Periodic one and a Quasi-Periodic material presenting long-range heterogeneities.

0.4.2 Periodic microstructures

Classically, architected materials are built with regular periodic lattices. Simple unique unit cells are usually tessellated periodically in space. This implicitly imposes

strong limitations on geometries of microstructures. Their periodicity also makes them prone to failure, as their tendency to split along definite structural planes is eased¹.

0.4.3 Quasi-Periodic microstructures

Quasi-periodic structures are well ordered structures that have no translational symmetry [Fleck et al., 2010, Wang and Sigmund, 2020]. They have been observed in many natural materials. The geometrical freedom they offer, i.e. over periodic distributions, provides a larger design space. In this work, focus will be drawn to [Penrose, 2013]’s kite&dart tiling (Figure 7(a)). *De facto*, the kite&dart tiling have regained interest after the discovery of atomistic samples with the same structures which makes this study more prone to answering the ever-growing interest from the scientific community. The geometrical aspect of the tiling is as follows: both the kite and dart are composed of two triangles each.

- The kite is a convex quadrilateral (72° , 144° , 72° , and 72°) that can be bisected to form two triangles (72° , 72° and 36°).
- The dart is a non-convex quadrilateral (36° , 216° , 36° , and 72°) that can be bisected along its axis of symmetry to form a pair of obtuse triangles (36° , 108° , and 36°).

Besides, this Kite&Dart Penrose lattice has a 5-fold symmetry leading to isotropic properties [Glacet, 2018] at the macroscopic scale^{2 3}.

We note the following interesting properties of the Quasi-Periodic lattice [Penrose, 2013]:

- Any pattern (of any size) can be found an infinite number of times in a lattice.
- Several patterns can coincide, however they are separated by regions that **do not** match.

0.4.4 Typical architectures of interest

As previously mentioned one Periodic and two Quasi-Periodic architected materials (microstructures) are investigated. The microstructures are based on a hexagonal (for the Periodic) and kite&dart Penrose (for the Quasi-Periodic) (see Figure 8). Both materials’

1. Drawing a parallel with material sciences (e.g. crystalline materials), such a process is called cleavage since it corresponds to successive and repeated breaking of bonds along specific ‘crystallographic’ plane.

2. A rotation by an angle of $(5 \times \frac{2\pi}{n})$ (rotation by 72° , 144° , 216° , 288° , 360° ,) does not change the object. (see e.g., Figure 7(b))

3. The isotropic property at the macroscopic scale is discussed further in Chapter 3.

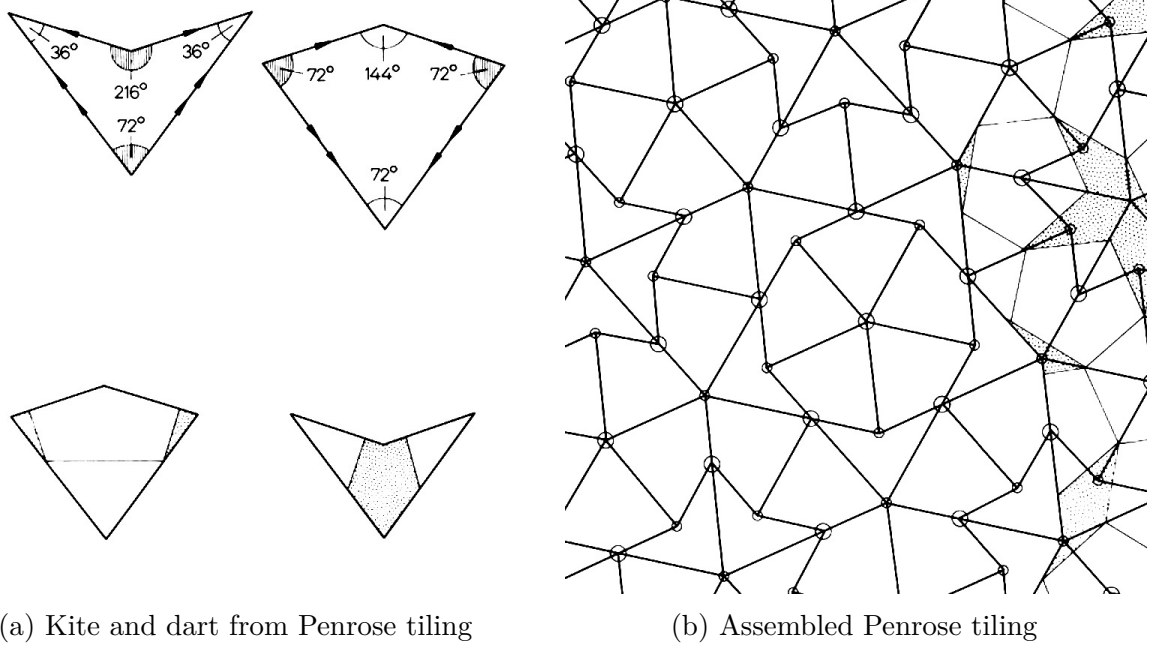
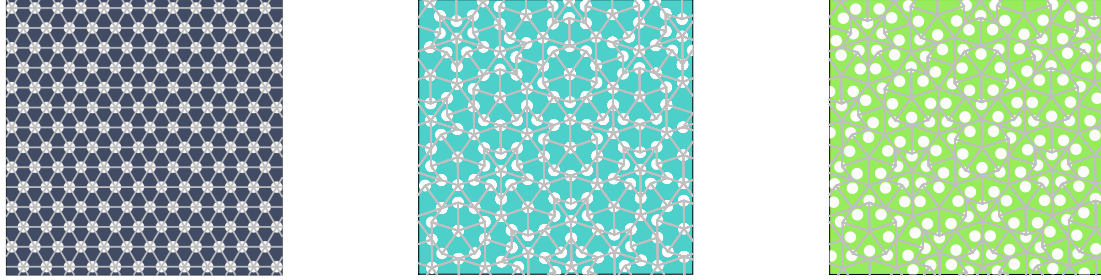


Figure 7 – Precise shapes of a Penrose kite&dart tiling and the assembled tiles [Penrose, 2013]

symmetry order (6 and 5-fold symmetry respectively) should lead to elastic isotropic equivalent media. We recall that for the hexagonal distribution, there's only one characteristic length of the microstructure that is the distance between holes, denoted by d ; while for the Penrose kite&dart paving, there are two characteristic length(s) corresponding to the opposite sides of the kite and/or dart quadrilateral d_k and d_d .

In order to meticulously compare the microstructures, the same hole radii r_h are taken, and the mean distances between the holes is fixed to $d = \text{mean}(d_k, d_d) = 4 \times r_h$ corresponding to a volume fraction of 78% for the hexagonal lattice and 75% for the Quasi-Periodic ones. The generated microstructures are shown in Figure 8, and their respective geometrical aspects are displayed in Table 1. Two types of Quasi-Periodic microstructures are considered, both based on the kite&dart Penrose paving. Type 1 corresponds to the holes drilled at the nodes of the paving, while type 2 suggests drilling holes at the centroids of the kites and darts in the paving, leading thus to same-yet-different perfectly controlled microstructures each one presenting specific Quasi-Periodic patterns. The different lengths and dimensions will be related to the characteristic length d for an easier perception and interpretation of the results.



(a) Periodic Hexagonal

(b) Quasi-Periodic - type 1

(c) Quasi-Periodic - type 2

Figure 8 – The microstructures considered for the study: a Periodic lattice of holes (a) and two types of Quasi-Periodic lattices of holes: distribution at the nodal positions of a kite&dart Penrose paving (type 1) (b) and on the centroids of the kite&dart paving (type 2) (c)

Typical microstructures properties		
Geometry	Characteristic length(s) (μm)	Hole radius (μm)
Periodic	3000	750
Quasi-Periodic - type 1	2270 and 3670	750
Quasi-Periodic - type 2	2270 and 3670	750

Table 1 – The microstructures and their geometrical aspects: The Periodic microstructure presents a unique characteristic length (the distance between the holes); while the Quasi-Periodic shows two [Penrose, 2013, Glacet, 2018]

0.5 Homogenisation techniques

The use of those highly heterogeneous architected materials is bridged by some limitations, *de facto*, treating the heterogeneities for accurately simulating the complex behaviour of such structures requires huge computational resources. Thus, of course, it's appealing to describe a simpler nature of those materials.

A variety of upscaling methods were proposed to reveal the relations between the microstructural heterogeneities from one side and the behaviour at higher scales from the other [Ongaro, 2018].

0.5.1 The presence of an *RVE*

The underlying principle of existing classical homogenisation techniques lies on the description of a structure with the help of a much smaller specimen, known as the representative volume element - *RVE*. This implicitly assumes the presence of two separated scales: (i) the microscopic scale that is small enough to capture the effects of the heterogeneities in the material, and (ii) the overall scale of the structure where the effects of the heterogeneities are expected to be smeared out, and on which effective material properties are considered [Michel et al., 1999]. The classical (first-order) homogenisation method is based on the construction of a boundary value problem on the *RVE* that allows the determination of the effective material properties at the higher scales [Ongaro, 2018]. In this case, the *RVE* should be big enough to statistically capture the heterogeneities and be constitutively valid, yet small enough to be considered as a volume element of continuum mechanics. More details on the classical homogenisation method can be found in the literature.

0.5.2 Limitations

The respective work outlines the following limitations: upscaled deformation modes of an *RVE* for a first-order homogenisation are linear; the first-order methods cannot take into account the size effects, nor large gradients of deformation, nor localisation, i.e., also, in case of large gradients, even materials with small microstructure cannot be accurately modelled [Geers et al., 2001]. Moreover, the first-order schemes do not work for softening materials. To surpass these problems, an extension to higher-order approaches has previously been addressed [Geers et al., 2001, Kouznetsova et al., 2002]. The solution

of the microscopic boundary-value problem in the case of higher-order computational homogenisation is effortless, yet allows for an enriched upscaled continuum with higher-order strain and stress-fields [Geers et al., 2001]. Although the higher-order techniques are able to treat softening materials, they present their limitations: localisation bands beyond a quadratic nature for the displacements cannot be resolved, e.g., softening materials in the presence of sharp localisation regions from the presence of a crack and/or high heterogeneities [Geers et al., 2010a].

As damage localises in narrow regions in a considered continuum, the length-scale that determines the variation of the defect falls below the considered scale of the mechanical fields (*RVE*) leading thus to what is known as gradient effects [Voyiadjis et al., 2004]. Gradient theories emerging from the multiscale nature of the mechanical framework are based on the enrichment of the classical continuum description with additional terms; those allow taking the gradient effects into account [Yang and Misra, 2010]. When the constitutive equations at the higher scales are difficult to write, general methods based on concurrent finite element simulations (FE2) can be applied [Feyel, 2003]. FE2 methods do not require any constitutive equations because all non-linearities come directly from the homogenisation of microscopic quantities after applying localisation rules to determine local solutions. Interests are presently concentrating on the development of a continuous-discontinuous homogenisation scheme, to allow the assessment of the presence of both micro and macro cracks, and where localisation bands are incorporated at the macroscale [Geers et al., 2010b]. Along the same line [Brancherie and Ibrahimbegovic, 2009] were able to describe microcracks by introducing a displacement discontinuity at the element level coupled with a continuum damage mechanics model, in parallel to assessing the failure process at the structure's level essentially due to the propagation of macro-cracks.

0.5.3 Recent advancement

Recently, work has been done on deriving a homogenised cohesive law at the macroscale from computations of crack propagation in a microscopic sample [Nguyen et al., 2011]. In [Loehnert and Belytschko, 2007], X-FEM approaches are used to incorporate the discontinuity at the macroscale, but as previous methods, this technique relies heavily on the principle of separation of scales as well as the presence of an *RVE* and it remains a homogenisation technique where a small part of the domain is considered to extract the full response of the structure; plus, both those methods rely on concurrent multilevel finite element (FE2) which is computationally expensive, and requires the difficult task of writing

a consistent homogenisation scheme to link the scales [Feyel, 2003]. Moreover, the need for enrichment of the description of the multiscale problem is directly perceived [Matous et al., 2008, Kulkarni et al., 2010, Hirschberger et al., 2009]. Although those methods are theoretically prominent, their experimental applicability remains questionable. In [Hossain et al., 2014], a different approach was proposed, where the effective toughness of the heterogeneous media was directly evaluated a priori (without concurrent computations). Recently, [Nguyen et al., 2019] followed the work of [Hossain et al., 2014] to identify the different parameters of a damage model at the mesoscale by fitting a typical force-displacement response on a heterogeneous structure. Yet, as the effective material properties are determined macroscopically from force-displacement responses, it's believed that micro-cracks and their influence on the structural responses fail to be taken into consideration.

0.5.4 The coarse-graining technique

The above mentioned methods stand as long as the separation of scales is prominent, or as long as an *RVE* can be well-defined, which naturally leads to a homogeneous description of the microstructures at the macroscopic scale. Nonetheless, when the microstructure's heterogeneities and/or the damage distribution are not statistically homogeneous, the effective description is expected to be dependent on the position in space and becomes influenced by simultaneous interactions between the damage and the microstructure. This restrains the above mentioned methods from accurately transferring the information from the microscopic scale to the macroscopic scale. Plus, to the authors' best knowledge, there's no available formulation allowing a consistent transfer of such information between the scales.

For this purpose, we follow the bottom-up approach of analysis in which information at the microscale is considered to inform the larger scales under the classical laws. We use a model-free coarse-graining technique [Goldhirsch and Goldenberg, 2002] - a widely used technique in Molecular Dynamics studies - where pseudo-molecular systems are built to reproduce physically consistent behaviour of all-atom with easier and faster computations. The coarse-graining technique [Goldhirsch and Goldenberg, 2002] is adapted to evaluate continuum mechanics at different intermediate mesoscales solely from the gathered data at the microscopic scale and by a manipulation of the inviolable conservation laws. This establishes effective fields of mechanical properties and opens the door for a better understanding of the relations between the scales.

The derivation of the proposed coarse-graining method is detailed in Chapter 2.

PART II

Computational approach: methods and implementation

PHASE-FIELD MODELLING OF BRITTLE FAILURE

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1.1 Introduction

As previously mentioned, one of the pillars of this work is the simulation of the failure process of architected materials at the microscopic scale, i.e., by explicitly taking the heterogeneities into account. The robustness and versatility of the phase-field model approach [Francfort, 1998, Bourdin et al., 2013, Wu et al., , Nguyen et al., 2015, Pham et al., 2017] regarding its independence of the finite element mesh and its ability to model complex scenarios (initiation, branching, coalescence, etc.) were decisive in its choice for the simulations.

The phase-field method is based on a diffuse representation of the localised discontinuity coming from the presence of a crack. A regularised variational principle describes the evolution of the mechanical problem from one side, and the evolution of an additional damage field α describing the damage state from the other. The typical Griffith's-type problems are rewritten in a variational framework [Francfort, 1998, Bourdin et al., 2008] leading to an energy functional resembling the potential presented by [Mumford and Shah, 1989]. Numerical implementation and some examples were provided in [Bourdin et al., 2000]. [Ambrosio and Tortorelli, 1990] proposed an approximation of this potential based on the theory of Γ -convergence. More recently, [Miehe et al., 2010a, Miehe et al., 2010b] have exploited the similarities with gradient-enhanced damage models and re-wrote phase-field models in a damage format by explicitly utilising notions like the degradation function, and the history function to set the irreversibility of damage. [Linse et al., 2017].

The overview of this chapter is as follows: first, the regularised representation of free discontinuities is introduced (Section 1.2), followed by an in-depth exhibition of the quasi-static (Section 1.3) and dynamic (Section 1.4) formulations of the phase-field problem. Two unilateral contact formulations are then discussed (Section 1.5). The computational and algorithmic frameworks based on the finite elements are put-forth (Section 1.6). In Sections 1.7 and 1.8, the influence of the regularisation parameter is displayed and most prominently, the role of the elastic threshold on the phenomenological behaviour is showcased. A validation of the phase-field implementation is complemented with a numerical study of the influence of the threshold along with the regularisation length on (i) the fracture of a uniaxial traction bar and on (ii) a dynamic crack branching benchmark (Section 1.9).

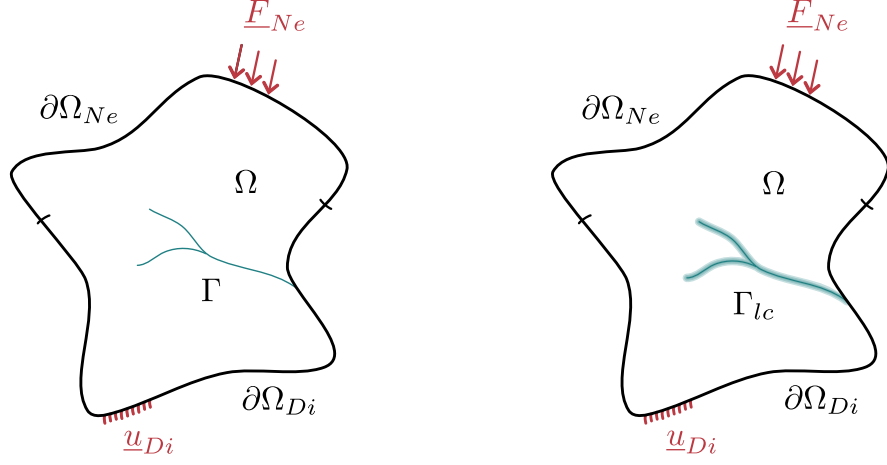


Figure 1.1 – Regularised representation of a crack in a two-dimensional case, sharp crack (left) and regularised representation through phase-field (right)

1.2 Regularised representation of free discontinuities

Consider a cracked body $\Omega \subset \mathbb{R}^D (D \in \{1, 2, 3\})$ under arbitrary external loads (Figure 1.1). D is the space dimension and $\partial\Omega$ the external boundary of the body. The displacement field of the body $\underline{u}(\underline{x}, t)$ should satisfy the Dirichlet boundary condition ($\underline{u}_{Di}$) applied on $\partial\Omega_{Di}$, and the stress field should satisfy the Neumann boundary condition ($\underline{F}_{Ne}$) on $\partial\Omega_{Ne}$. Let Γ , a curve of dimension $D - 1$ within Ω , hold an internal discontinuity, i.e., a crack. Within a regularised framework, the cracks in the phase-field models are approximated by bands of finite thickness of a continuous phase-field variable $\alpha(\underline{x})$ known as the damage field: $\alpha(\underline{x})$ describes the material damage state, i.e., it takes the value 0 in the intact region of the material and $0 < \alpha \leq 1$ to represent the smeared crack. It's shown (see e.g. [Miehe et al., 2010b, Miehe et al., 2010a]) that the damage field can be determined by solving the following boundary value problem in Ω :

$$\begin{aligned} \alpha - l_c^2 \Delta \alpha &= 0 & \text{in } \Omega \\ \alpha(x) &= 1 & , \text{ on } \Gamma \\ \nabla \alpha(\underline{x}) \cdot \underline{n} &= 0 & \text{on } \partial\Omega \end{aligned} \tag{1.1}$$

where $\Delta(\cdot)$ is the Laplacian, $\underline{n}$ the outward normal to $\partial\Omega$, l_c is a length describing the actual width of the regularised crack. Refer to Figure 1.1 for a two-dimensional illustration of this problem. The Euler-Lagrange Equation of Equation (1.1) is associated with the

following variational problem [Nguyen et al., 2017]:

$$\begin{aligned}\alpha(\underline{x}) &= \arg\left\{\inf_{\alpha \in L_\alpha} \Gamma_{l_c}(\alpha)\right\}, \\ \text{with } L_\alpha &= \{\alpha | \alpha(\underline{x}) = 1 \text{ on } \Gamma, \forall \underline{x} \in \Gamma\} \text{ and where} \\ \Gamma_{l_c}(\alpha) &= \int_{\Omega} \gamma(\alpha, \nabla \alpha, l_c) d\Omega \text{ represents the total crack length.}\end{aligned}\tag{1.2}$$

Various geometric crack functions $\gamma(\alpha, \nabla \alpha, l_c)$ (or crack density functions) can be found in the literature. In this study, the quadratic crack surface density function following [Miehe et al., 2010a] is considered¹ :

$$\gamma(\alpha, \nabla \alpha, l_c) = \frac{1}{2l_c} \alpha^2 + \frac{l_c}{2} \nabla \alpha \bullet \nabla \alpha \tag{1.3}$$

It's recalled that the crack density function $\gamma(\alpha, \nabla \alpha, l_c)$ smears-out the crack by introducing a length parameter l_c ². The term in α^2 represents the local part and the second term denotes the non-local part incorporating l_c . Combining Equation (1.2) and (1.3), the phase-field damage variable $\alpha(\underline{x})$ becomes the solution of the following variational problem [Nguyen et al., 2017]:

$$\alpha(\underline{x}) = \arg\left\{\inf_{\alpha \in L_\alpha} \int_{\Omega} \gamma(\alpha, \nabla \alpha, l_c) d\Omega \right\}. \tag{1.4}$$

The crack surface density function γ along with the phase-field damage variable α are consequently considered to approximate the crack by a smeared representation. In the next sections, the quasi-static and the dynamic formulations are introduced respectively.

1.3 Quasi-static formulation of the phase-field model

As the phase-field model can be seen as a variational formulation of a Griffith-like problem, we start by recalling Griffith's theory of quasi-static brittle failure; we then display its variational formulation.

Griffith proposed an energy-based criterion for a straight crack propagating in an infinite homogeneous plane subjected to uniform tensile stress. According to the theory of brittle fracture, the energy required to create a unit area of the fracture surface is equal to a

1. A brief discussion on the choice regarding the crack density function is presented in Paragraph 1.2.

2. The length parameter has been previously assessed in [Borden et al., 2012, Nguyen et al., 2016]. More details are found in Section 1.7

critical fracture energy density g_c also known as the critical energy release rate. Assuming small strains, [Francfort, 1998, Bourdin et al., 2008] proposed a variational approach with the following energy functional for a cracked body based on the Griffith criterion:

$$E(\underline{u}, \Gamma) = E_u(\underline{u}, \Gamma) + E_s(\Gamma) - E_e(\underline{u}) \quad (1.5)$$

$E_e(\underline{u})$ is the external potential energy, i.e., the work of external forces on $\underline{u}$, given by $E_e(\underline{u}) = \int_{\Omega} \underline{f} \cdot \underline{u} d\Omega + \int_{\Omega_{Ne}} \underline{F}_{Ne} \cdot \underline{u} d\Omega_{Ne}$, $\underline{f}$ corresponds to a given body force and $\underline{F}_{Ne}$ to a load applied to Ω_{Ne} . $E_u(\underline{u}, \Gamma)$ is the strain energy stored in the cracked body, $E_s(\Gamma)$ is the energy required to create the crack according to Griffith Criterion - known as the fracture energy. To circumvent the numerical problems associated with the propagating discontinuity Γ (the crack set), the discontinuity is approximated by a function written in terms of a continuous damage field α (Section 1.2), known as the phase field. The function $\Gamma_{l_c}(\alpha) = \int_{\Omega} \gamma(\alpha, \nabla \alpha, l_c) d\Omega$ (Section 1.2) can reasonably be considered. It's recalled that the continuous phase-field variable α describes the material damage state, i.e., it takes the value 0 in the intact region of the material and $0 < \alpha \leq 1$ to represent the smeared crack (of width l_c). Due to the phase-field regularisation, the stored strain energy $E_u(\underline{u}, \Gamma)$ depends not only on $\underline{u}$, but also on the crack phase-field α . $E_u(\underline{u}, \alpha)$ underlines thus zones of deterioration of the material ($0 < \alpha \leq 1$). Equation (1.5) becomes:

$$\begin{aligned} E(\underline{u}, \alpha) &= E_u(\underline{u}, \alpha) + E_s(\alpha) - E_e(\underline{u}) \\ &= \int_{\Omega} W(\underline{\varepsilon}(\underline{u}), \alpha) d\Omega = \int_{\Omega} W_u(\underline{\varepsilon}(\underline{u}), \alpha) d\Omega + g_c \int_{\Omega} \gamma(\alpha, \nabla \alpha) d\Omega - E_e(\underline{u}) \end{aligned} \quad (1.6)$$

The term $W(\underline{\varepsilon}(\underline{u}), \alpha)$ denotes the total energy density. The term $W_u(\underline{\varepsilon}(\underline{u}), \alpha)$ represents the strain energy density in the deteriorated body ($0 \leq \alpha \leq 1$). $\underline{\varepsilon}$ is the displacement symmetric gradient. To link the mechanical fields (displacement $\underline{u}$, stresses $\underline{\sigma}, \dots$) to the damage phase-field (α), different energetic degradation functions $g(\alpha)$ were considered in the literature, the most common one being $g(\alpha) = (1 - \alpha)^2$ (See paragraph 1.4 for more details). By assuming that the damage occurs equivalently in tension and compression, the deterioration of the initially elastic strain energy density $W_u(\underline{\varepsilon}(\underline{u})) = \frac{1}{2} \underline{\sigma} : \underline{\varepsilon} = \frac{1}{2} \underline{\varepsilon} : \mathbb{C} : \underline{\varepsilon}$ can be expressed as follows: $W_u(\underline{\varepsilon}(\underline{u}), \alpha) = g(\alpha) W_u(\underline{\varepsilon}(\underline{u}))$. $\mathbb{C}$ is the standard sound isotropic

Hooke's elasticity tensor. Equation (1.6) reads:

$$E(\underline{u}, \alpha) = \int_{\Omega} g(\alpha) \left(\frac{1}{2} \boldsymbol{\varepsilon} : \mathbb{C} : \boldsymbol{\varepsilon} \right) d\Omega + g_c \int_{\Omega} \gamma(\alpha, \nabla \alpha) d\Omega - E_e(\underline{u}) \quad (1.7)$$

Veritably, damage occurs more easily in tension than in compression, thus tension-compression asymmetry formulations are needed [Amor et al., 2009, Miehe et al., 2010a, He and Shao, 2019]. The elastic strain energy of the deteriorated material is written as $W_u(\boldsymbol{\varepsilon}(\underline{u}, \alpha)) = g(\alpha) W_u^+(\boldsymbol{\varepsilon}(\underline{u})) + W_u^-(\boldsymbol{\varepsilon}(\underline{u}))$, where $W_u^+(\boldsymbol{\varepsilon}(\underline{u}))$ and $W_u^-(\boldsymbol{\varepsilon}(\underline{u}))$ denote the positive (active) and negative (passive) parts of the strain energy of the sound material. Check Section 1.5 for more details regarding the different types of the energy split.

Evolution of phase-field: basics of thermodynamics

By applying the second law of thermodynamics, the thermodynamical allowance of the constitutive relation is examined [Miehe et al., 2010b, Nguyen et al., 2017]. Assuming isothermal process, the Clausius-Duhem inequality states:

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{W} \geq 0, \quad (1.8)$$

where $\boldsymbol{\sigma}$ corresponds to the standard Cauchy stress. Equation (1.8) can be rewritten as:

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{W} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \frac{\partial W}{\partial \boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}} - \frac{\partial W}{\partial \alpha} \dot{\alpha} = \left(\boldsymbol{\sigma} - \frac{\partial W}{\partial \boldsymbol{\varepsilon}} \right) : \dot{\boldsymbol{\varepsilon}} - \frac{\partial W}{\partial \alpha} \dot{\alpha} \geq 0 \quad (1.9)$$

This inequality should be satisfied for any process; if one considers a process without damage evolution ($\dot{\alpha}=0$), then there is no dissipation, and the inequality becomes an equality ($\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \dot{W} = 0$) allowing the definition of the constitutive relation as:

$$\boldsymbol{\sigma} = \frac{\partial W}{\partial \boldsymbol{\varepsilon}}. \quad (1.10)$$

Next, a crack phase-field evolution is formulated guaranteeing the irreversibility of the process. A reduced form of Equation (1.8) reads:

$$\mathcal{A} \dot{\alpha} \geq 0 \quad (1.11)$$

where $\mathcal{A}$ is the variational derivative of $W(\boldsymbol{\varepsilon}(\underline{u}), \alpha)$ with respect to the phase-field variable

α :

$$\mathcal{A} = -\frac{\delta W}{\delta \alpha} = -\frac{\partial W}{\partial \alpha} + \nabla \cdot \left(\frac{\partial W}{\partial \nabla \alpha} \right), \quad (1.12)$$

$\mathcal{A}$ can be seen as the thermodynamic force associated with α . A threshold function $F(\mathcal{A})$ such as no damage occurs should then satisfy the following condition (constraint):

$$F(\mathcal{A}) \leq 0 \quad (1.13)$$

The principle of maximum dissipation requires the dissipation $\mathcal{A}\dot{\alpha}$ to be maximal under the constraint (1.13). This yields the following Lagrangian:

$$\mathfrak{L} = -\mathcal{A}\dot{\alpha} + \lambda_L F(\mathcal{A}), \quad (1.14)$$

that satisfies the Kuhn-Tucker conditions as:

$$\frac{\partial \mathfrak{L}}{\partial \mathcal{A}} = 0, \lambda_L \geq 0, F \leq 0, \lambda_L F = 0 \quad (1.15)$$

The first inequality in Equation (1.15) gives:

$$\dot{\alpha} = \lambda_L \frac{\partial F(\mathcal{A})}{\partial \mathcal{A}} \quad (1.16)$$

Assuming $F(\mathcal{A}) = \mathcal{A}$, one obtains $\dot{\alpha} = \mathcal{L} \geq 0$.

Subsequently, from ($\dot{\alpha} \geq 0$ and $F(\mathcal{A}) = \mathcal{A}$), from the third inequality in (1.15) ($F \leq 0$), and from the inequality (1.11) ($\mathcal{A} \dot{\alpha} \geq 0$), the functional F becomes null, and the following Equation is obtained:

$$F = \mathcal{A} = -\frac{\delta W}{\delta \alpha} = 0 \quad (1.17)$$

Ultimately, the displacement and phase-fields $(\underline{u}, \alpha)$ are computed by solving the following minimisation problem:

$$(\underline{u}, \alpha) = \arg\{\min(E(\underline{u}, \alpha))\} \text{ subjected to } \dot{\alpha} \geq 0 \text{ and } 0 \leq \alpha \leq 1 \quad (1.18)$$

As seen, a non-reversible evolution of the damage phase-field is satisfied, while the bound-ness is to be imposed. Practically, the coupling of the mechanical $\underline{u}$ and the damage α problems leads to convergence issues for the solution as the coupled problems appears to be non-convex.

By introducing a history function $\mathcal{H}$ (also claimed to take care of the probable load-

ing/unloading [Molnár et al., 2020a]), [Miehe et al., 2010a, Miehe et al., 2010b] decoupled the problems and allowed for a simple alternating minimisation (staggered) solution following :

$$\begin{aligned} \underline{u} &= \arg\{\inf_{\underline{u}} [\int_{\Omega} g(\alpha) W_u(\underline{\epsilon}(\underline{u})) - \underline{f} \cdot \underline{u}] d\Omega - \int_{\Omega_{Ne}} \underline{F}_{Ne} \cdot \underline{u} d\Omega_{Ne}\} \\ \alpha &= \arg\{\inf_{\alpha} \int_{\Omega} [g_c \gamma(\alpha, \nabla \alpha, l_c) + g(\alpha) \mathcal{H}] d\Omega\} \end{aligned} \quad (1.19)$$

while naturally accounting for the positivity of the damage rate. The history function $\mathcal{H}$ represents 'the maximum strain energy obtained in the deformation history of a material point', it can be considered as a measure of the maximum active (tensile) part of the strain energy, i.e., W_u^+ obtained in history.[Miehe et al., 2010a]. At a time $t = t_0$, it can be expressed as:

$$\mathcal{H}^{t=t_0} = \max(\mathcal{H}^{t < t_0}, W_u^{+, t=t_0}) \text{ with } \mathcal{H}^0 = 0 \quad (1.20)$$

More info about Miehe's history function $\mathcal{H}$ and other proposed methods are briefly stated in Paragraph 1.3

§ 1.1. On the length scale l_c

It was shown that this phase-field modelling approach converges to the classical brittle failure when the regularisation parameter l_c approaches 0. The length parameter l_c is widely regarded as a material parameter [Pham et al., 2011a, Nguyen et al., 2016, Linse et al., 2017, Wu et al.,]. In fact, [Nguyen et al., 2016] -between others-, elaborated analytical expressions linking the length scale parameter l_c to other material parameters, namely g_c , the critical stress σ_c (maximum stress state reached before softening) and the elastic modulus (E)³. Even though the formula for l_c is determined for a unidimensional bar with homogeneous damage field, it was shown that the expressions stand for 2D/3D samples with notches when l_c is small enough compared with the problem's characteristic dimensions [Mesgarnejad et al., 2015, Zhang et al., 2017].

§ 1.2. On the crack density function γ

The herein considered crack density function is one of the most commonly used, as the solution algorithm can be implemented in any standard finite element solver. The absence of an initial elastic threshold (due to the quadratic nature of the crack surface function) has lead some authors [Nguyen et al., 2017] to add an artificial initial elastic threshold (e.g., $\phi_c = \frac{g_c}{2l_c}$). This threshold ensured that no damage occurs at low stress-strain levels.

3. Refer to Section 1.7 for a detailed development of the expressions.

Explicitly, this energy threshold was added to the history function $\mathcal{H}$. The reader is referred to Paragraph 1.3 for further details.

Further along, [Pham et al., 2011b] proposed a crack surface density function with a linear term, knowingly $\gamma(\alpha, \nabla\alpha) = \frac{3}{8l_c}\alpha + \frac{3l_c}{8}\nabla\alpha \bullet \nabla\alpha$. This crack density function allows for the phenomenological behaviour to remain elastic until the maximum stress state is reached (as opposed to the quadratic crack density function where the elasticity is degraded before reaching the maximum stress). However, in this case, the natural lower bound of the damage variable $\alpha \geq 0$ is violated and bound-constrained optimisation techniques are needed. We will restrain our work to the quadratic crack surface density function undertaking its limitations.

§ 1.3. On the history function $\mathcal{H}$

When implementing a phase-field model, the boundedness $0 \leq \alpha \leq 1$ and the irreversibility conditions $\dot{\alpha} \geq 0$ must be guaranteed. Moreover, it was seen that the solution of the fully coupled problem suffers from non-convexity [Miehe et al., 2010a, Miehe et al., 2010b]. Multiple methods are proposed [Molnár et al., 2020a] to overcome these issues, e.g., bound-constrained non-linear optimisation techniques, augmented Lagrangian or penalisation methods. However, [Miehe et al., 2010a, Miehe et al., 2010b] proposed a one-pass staggered algorithm using a local history variable, applicable to the standard phase-field modelling algorithm with the quadratic geometric function γ . The history function $\mathcal{H}$ represents 'the maximum strain energy obtained in the deformation history of a material point, which may be considered as a measure for the maximum tensile strain obtained in history.' When an initial elastic threshold is added, it ensures that the strain energy remains null as long as the energy threshold is not surpassed. A modification of Equation (1.20) can be expressed as follows:

$$\mathcal{H}_c^{t=t_0} = \max(\mathcal{H}_c^{t<t_0}, W_u^{+,t=t_0} - \phi_c) \text{ with } \mathcal{H}_c^0 = 0 \quad (1.21)$$

The modified history function $\mathcal{H}_c$ is equal to zero when the strain energy is below the threshold ϕ_c , prohibiting thus damaging at low strains. It's noted that the threshold is implemented such that in case of absence of damage, the elastic behaviour is recovered [Nguyen et al., 2017, Molnár et al., 2020b]. The total energy density (Equation 1.7) is re-written as:

$$\int_{\Omega} W(\underline{\varepsilon}(\underline{u}), \alpha) d\Omega = \int_{\Omega} g(\alpha)(W_u(\underline{\varepsilon}(\underline{u})) - \phi_c) d\Omega + \phi_c + g_c \int_{\Omega} \gamma(\alpha, \nabla\alpha) d\Omega - E_e(\underline{u}) \quad (1.22)$$

Leading then to a reformulation of the staggered problem (Equation (1.19)):

$$\begin{aligned} \underline{u} &= \arg\{\inf_{\underline{u}} [\int_{\Omega} g(\alpha) W_u(\underline{\epsilon}(\underline{u})) - \underline{f} \cdot \underline{u}] d\Omega - \int_{\Omega_{Ne}} \underline{F}_{Ne} \cdot \underline{u} d\Omega_{Ne}\} \\ \alpha &= \arg\{\inf_{\alpha} [\int_{\Omega} [g_c \gamma(\alpha, \nabla \alpha, l_c) + g(\alpha) \mathcal{H}_c] d\Omega + \phi_c]\} \end{aligned} \quad (1.23)$$

This formulation verifies that for no damage, the classical form of the elastic behaviour of the material is recovered. Although there is no clear mathematical proof of how this herein introduced history function $\mathcal{H}/\mathcal{H}_c$ enforces damage irreversibly, the numerical examples and studies show no violation of this criterion [Linse et al., 2017, Molnár et al., 2020a], moreover, the simplicity of this method and its ease of implementation played a major role in its widespread in the community. It's noted that in the following, $\mathcal{H}$ and $\mathcal{H}_c$ will be used when addressing the classical and the modified versions (with threshold) of the history function respectively.

§ 1.4. On the degradation function $g(\alpha)$

The energetic degradation function $g(\alpha)$ links the mechanical fields, i.e., strain energy, stress., to the damage phase-field α ; it's borrowed from damage mechanics concepts. Different energetic degradation function $g(\alpha)$ were considered in the literature, the most common one being $g(\alpha) = (1 - k)(1 - \alpha)^2 + k \simeq (1 - \alpha)^2$. The parameter k is a small numerical parameter introduced in the degradation to ensure the well-conditioning of the system of equations. Any degradation function should satisfy (i) that the material is initially undamaged $g(\alpha = 0) = 1$ and that (ii) the fully damaged material stores no elastic strain energy $g(\alpha = 1) = 0$. (iii) $g(\alpha)$ should be a monotonically decreasing function to represent the deterioration of the material and (iv) $\frac{dg}{d\alpha(1)} = 0$. The fourth condition guarantees that the strain energy density function takes a finite value in a locally cracked domain [Wu et al., 2020, Brides, 1998], and ensures that the localisation band does not grow orthogonally [Borst and Brekelmans, 1996].

Remark 1.1. In $g(\alpha) = (1 - \alpha)^2$, the damage variable α does not correspond to the damage in the classical sense of damage mechanics [Bažant and Jirásek, 2002] (see the introductory Chapter 0, where a softening constitutive law $\underline{\sigma} = (1 - D)\mathbb{C}\underline{\epsilon}$ is introduced). But of course, parallels can be drawn and D and α are easily interlinked.

In this section the main ingredients of the quasi-statics phase-field modelling of brittle failure are reviewed. In the next section, the variational ingredients of Griffith's theory for dynamic brittle fracture are recalled, and the phase-field approximation of dynamic brittle

fracture with the governing equations are put-forth.

1.4 Dynamic formulation of the phase-field model

In Section 1.3, the analysis focuses on the quasi-static failure of brittle material neglecting thus inertial effects. Here, the variational ingredients of the dynamic phase-field model are presented. Similarly to the quasi-static case, energy dissipation comes solely from the damaging process. Starting with a two-dimensional isotropic body Ω , under small strains assumptions, [Li et al., 2016a] writes the total energy of the body as:

$$\begin{aligned} E(\underline{u}, \underline{\dot{u}}, \Gamma) &= E_u(\underline{u}, \Gamma) + E_k(\underline{\dot{u}}) + E_s(\Gamma) - E_e(\underline{u}) \\ &= \int_{\Omega} W_u(\underline{\varepsilon}(\underline{u}), \alpha) d\Omega + \int_{\Omega} K_{\dot{u}}(\underline{\dot{u}}) d\Omega + g_c \int_{\Omega} \gamma(\alpha, \nabla \alpha) d\Omega - E_e(\underline{u}) \end{aligned} \quad (1.24)$$

where $E_k(\underline{\dot{u}})$ corresponds to the total kinetic energy of the body, mass conservation is admitted and the material degradation is assumed to have no influence on the local material density. This leads to the classical definition of the kinetic energy density being $K_{\dot{u}} = \frac{1}{2} \rho \dot{\underline{u}} \cdot \underline{\dot{u}}$, with ρ the mass density of the material, and $\underline{\dot{u}} = \frac{\partial \underline{u}}{\partial t}$. The problem reduces to formulate the displacement-damage evolution as a boundary value problem following Hamilton's principle [Li et al., 2016a]. Over an arbitrary interval of time $\mathfrak{T} = [0, T]$, an action-integral is introduced as follows:

$$\mathfrak{A}(\underline{u}, \underline{\dot{u}}, \alpha) = \int_{\mathfrak{T}} E_u(\underline{u}, \alpha) + E_s(\alpha) - E_k(\underline{\dot{u}}) - E_e(\underline{u}) dt \quad (1.25)$$

governed by the following principles:

- **Damage irreversibility:** $\dot{\alpha} \geq 0 \ \forall t \text{ in } \mathfrak{T}$;
- **First order stability:** $\mathfrak{A}'(\underline{u}, \underline{\dot{u}}) \geq 0$ of admissible displacements and damage evolution;
- **Energy balance:** $E_s(\alpha)$ is responsible of the energy dissipation in the system;

The evaluation of the directional (Gâteaux) derivative of the action integral leads to the following weak elastic-damage dynamic wave equation:

$$\underline{\text{div}} \underline{\sigma} + \underline{f} = \rho \underline{\ddot{u}} \quad (1.26)$$

with appropriate boundary conditions where $\underline{f}$ corresponds to a given body force density. In comparison with the classical elastodynamic solution, the stress state $\boldsymbol{\sigma}$ is modulated by the degradation function $g(\alpha)$ due to deterioration of the material following $\boldsymbol{\sigma} = g(\alpha)\mathbb{C}:\boldsymbol{\varepsilon}$. Moreover, the total energy satisfies a minimum principle constrained by the irreversibility of the damage:

$$E_u(\underline{u}^t, \alpha^t) + E_s(\alpha^t) \leq E_u(\underline{u}^{t+}, \alpha^{t+}) + E_s(\alpha^{t+}) \quad (1.27)$$

The superscript t and $t+$ refers to quantities evaluated at time t and $t+$ respectively. $t+ \geq t$. Here, the displacement field evolution is governed by the damage-dynamic-wave (Equation (1.26)). Practically, at each time step, damage-dynamic-wave equation is solved to compute the updated displacement field $\underline{u}$ while Equation (1.27) is solved for the damage field α (See section 1.6 for more details on the overall algorithm).

After introducing both the quasi-static and dynamic phase-field model, and before displaying their overall algorithms, we summarise in the next section the tension-compression asymmetry formulations needed to split the positive (active) and negative (passive) parts of the strain.

1.5 Unilateral contact formulations

In order to prevent the issue of crack interpenetration in compression mode, and to account for the tension-compression asymmetry observed in brittle materials, many unilateral contact formulations have been proposed in the literature [Freddi and Royer-Carfagni, 2010]. Damage occurs more easily in tension than in compression, and tension-compression asymmetry formulations are much needed. This asymmetry is usually translated as a split of the elastic strain density function into a damaging (tension) part W_u^+ , and a compression part W_u^- which does not activate damage. The strain energy of a sound body is hence written as:

$$W_u(\boldsymbol{\varepsilon}(\underline{u})) = W_u^+(\boldsymbol{\varepsilon}(\underline{u})) + W_u^-(\boldsymbol{\varepsilon}(\underline{u})) \quad , \quad (1.28)$$

while for a deteriorated body, the split translates to:

$$W_u(\boldsymbol{\varepsilon}(\underline{u}, \alpha)) = g(\alpha)W_u^+(\boldsymbol{\varepsilon}(\underline{u})) + W_u^-(\boldsymbol{\varepsilon}(\underline{u})) \quad (1.29)$$

Several formulations for the decomposition to positive/negative parts are proposed [Amor et al., 2009, Miehe et al., 2010a, He and Shao, 2019]. In this study we focus on two

formulations: the extensive/compressive decomposition [Miehe et al., 2010a], and a new formulation based on the orthogonal decomposition of the strain into two complementary parts [He and Shao, 2019], which are orthogonal in the sense of an inner product, where $\mathbb{C}$ acts as a metric operator [Nguyen et al., 2020a]. The more common extensive-compressive formulation is considered in the quasi-static case, while the orthogonal more 'clean' decomposition is considered in the dynamic algorithm where compressive and tensile wave reflections occur.

1.5.1 Extensive/compressive decomposition of the strain

In [Miehe et al., 2010a], the formulation is based on the spectral decomposition of the strain tensor into negative (compressive, inactive) and positive (tensile, damageable) parts.

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^+ + \boldsymbol{\varepsilon}^- \quad (1.30)$$

The tensile/compressive contributions correspond to the positive/negative parts of the principal strains written $\boldsymbol{\varepsilon}^i = \sum_i \varepsilon^i \mathbf{n}^i \otimes \mathbf{n}^i$. where ε^i denote the principal strains and $\mathbf{n}^i$ the corresponding principal directions. The decomposition writes:

$$\begin{aligned} \boldsymbol{\varepsilon} &= \boldsymbol{\varepsilon}^+ + \boldsymbol{\varepsilon}^- \\ &= \sum_i \langle \varepsilon^i \rangle^+ \mathbf{n}^i \otimes \mathbf{n}^i + \sum_i \langle \varepsilon^i \rangle^- \mathbf{n}^i \otimes \mathbf{n}^i \end{aligned} \quad (1.31)$$

where the bracket operators denote $\langle \cdot \rangle^+ = (\cdot + |\cdot|)/2$, and $\langle \cdot \rangle^- = (\cdot - |\cdot|)/2$, i.e., $\langle \cdot \rangle^+ = \cdot$ if $\cdot > 0$ and $\langle \cdot \rangle^+ = 0$ if $\cdot < 0$, while $\langle \cdot \rangle^- = \cdot$ if $\cdot < 0$ and $\langle \cdot \rangle^- = 0$ if $\cdot > 0$. The damage is then assumed to be created by traction (the positive part) only, and the strain energy density decomposition reads:

$$W_u^{+/-}(\boldsymbol{\varepsilon}(\underline{u})) = \frac{\lambda}{2} [\langle \text{tr} \boldsymbol{\varepsilon} \rangle^{+/-}]^2 + \mu \text{tr}[(\boldsymbol{\varepsilon}^{+/-})^2] \quad (1.32)$$

λ and μ are the corresponding Lamé elastic parameters of the sound material. It's mentioned that the spectral decomposition of the strain tensor induces strong nonlinearity for the mechanical solution. The shifted strain tensor split algorithms is followed [Nguyen et al., 2015]. Another limitation of this decomposition is that it's only able to simulate damage in initially isotropic elastic materials, and has no extension to the anisotropic case according to [Nguyen et al., 2020b].

1.5.2 Orthogonal decomposition of strain

An alternative formulation is based on the orthogonal decomposition of the strain into two complementary parts [He and Shao, 2019], that are orthogonal in the sense of an inner production where the elastic stiffness tensor $\mathbb{C}$ acts as a metric operator. The strain energy density decomposition is expressed as:

$$W_u^{+/-}(\boldsymbol{\varepsilon}(\underline{u})) = \frac{1}{2}[\boldsymbol{\varepsilon}^{+/-} : \mathbb{C} : \boldsymbol{\varepsilon}^{+/-}] \quad (1.33)$$

As the negative/positive parts of the energy depend directly on the stiffness tensor $\mathbb{C}$, the extension of this method to initially anisotropic elastic materials is straightforward. The orthogonality condition satisfies

$$\boldsymbol{\varepsilon}^+ : \mathbb{C} : \boldsymbol{\varepsilon}^- = 0 = \boldsymbol{\varepsilon}^- : \mathbb{C} : \boldsymbol{\varepsilon}^+ \quad (1.34)$$

[He and Shao, 2019] proposed a method to impose the orthogonality condition (Equation (1.34)). A brief summary is presented here: first, the square-root of the elastic tensor $\mathbb{C}$ is introduced via:

$$\mathbb{C}^{1/2} = \sum_i C_i^{1/2} \mathbf{n}^i \otimes \mathbf{n}^i \text{ and } \mathbb{C}^{-1/2} = \sum_i C_i^{-1/2} \mathbf{n}^i \otimes \mathbf{n}^i, \quad (1.35)$$

where C^i are the eigenvalues of $\mathbb{C}$, and $\mathbf{n}^i$ are second-order orthonormal eigentensors associated to C^i . In the case of isotropic case, the square roots of the elastic tensor are specified by:

$$\mathbb{C}^{1/2} = \begin{bmatrix} \sqrt{\frac{\kappa}{2}} + \sqrt{\frac{\mu}{2}} & \sqrt{\frac{\kappa}{2}} - \sqrt{\frac{\mu}{2}} & 0 \\ \sqrt{\frac{\kappa}{2}} - \sqrt{\frac{\mu}{2}} & \sqrt{\frac{\kappa}{2}} + \sqrt{\frac{\mu}{2}} & 0 \\ 0 & 0 & \sqrt{2\mu} \end{bmatrix} \text{ and } \mathbb{C}^{-1/2} = \begin{bmatrix} \frac{1}{2\sqrt{2\kappa}} + \frac{1}{2\sqrt{2\mu}} & \frac{1}{2\sqrt{2\kappa}} - \frac{1}{2\sqrt{2\mu}} & 0 \\ \frac{1}{2\sqrt{2\kappa}} - \frac{1}{2\sqrt{2\mu}} & \frac{1}{2\sqrt{2\kappa}} + \frac{1}{2\sqrt{2\mu}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2\mu}} \end{bmatrix} \quad (1.36)$$

where κ is the bulk modulus. It's noted that the computation of the square-root of $\mathbb{C}$ is done only once, as it corresponds to the sound material. Following [Nguyen et al., 2020b], the transformed strain tensor is defined as $\tilde{\boldsymbol{\varepsilon}} = \mathbb{C}^{1/2} : \boldsymbol{\varepsilon}$. A spectral decomposition is applied on the transformed strain tensor $\tilde{\boldsymbol{\varepsilon}}$ in this new space as

$$\tilde{\boldsymbol{\varepsilon}} = \tilde{\boldsymbol{\varepsilon}}^+ + \tilde{\boldsymbol{\varepsilon}}^-, \text{ where } \tilde{\boldsymbol{\varepsilon}}^{+/-} = \sum_i \langle \tilde{\boldsymbol{\varepsilon}}^i \rangle^{+/-} \mathbf{n}^i \otimes \mathbf{n}^i \quad (1.37)$$

$\tilde{\epsilon}^i$ are the principal tranformed strains and $\mathbf{n}^i$ their corresponding orthogonal principal directions. The brackets are defined in Section 1.5.2. The split in the problem's space is obtained once the split of the transformed strains is computed following

$$\epsilon^{+/-} = \mathbb{C}^{-1/2} : \tilde{\epsilon}^{+/-} \quad (1.38)$$

The herein obtained negative/positive parts of the strain tensor satisfy the orthogonality condition since $\epsilon^+ : \epsilon^- = 0$ [He and Shao, 2019]. Similarly to [Miehe et al., 2010a], the decomposition of the strain tensor induces strong non-linearity for the mechanical solution and requires numerical treatment for efficiency. However, since the choice of the split is only considered for the dynamic problem, and since the dynamic-wave equation is solved explicitly, this non-linearity does not affect the mechanical problem; and the split can be efficiently implemented for the dynamic phase-field problem.

1.6 Overall phase-field algorithms: implementation and numerical simulation method

1.6.1 Staggered procedure for quasi-static phase-field model

In this section, the above reported quasi-static phase-field model is numerically described. In the quasi-static case, the time steps t^n refer to the load increment. Time stepping and adaptive load increments are studied in the literature [Nguyen et al., 2015]. Here, fixed time steps (hence load increments) are considered. The following box summarizes the overall algorithm of the quasi-static phase-field model. $\mathcal{H}_c$ and $\mathcal{H}$ are interchangeable in the algorithm, to take (or not) an elastic threshold into account.

Staggered procedure for quasi-static phase-field model

Initialise $\underline{u}^0$, α^0 and $\mathcal{H}_c^0 = 0$

while $t^n \leq T$, given $\underline{u}^n$, α^n and $\mathcal{H}_c^n$

1. Compute the history function $\mathcal{H}_c^{n+1}$ from Equation (1.21) ($\underline{u}^n$)
2. Compute the damage phase-field α^{n+1} by solving the linear phase-field problem (Equation (1.23)) at fixed displacement field $\underline{u}^n$
3. Compute the displacement field $\underline{u}^{n+1}$ via the staggered solving algorithm at fixed damage field α^{n+1} (Equation (1.23))
4. $n = n + 1$ and go to 2

A classical linear FE implementation is considered. The ideal properties of spatial discretisation are chosen following [Nguyen et al., 2016]. The mesh size h is usually taken approximately $h \simeq l_c/3$ to $l_c/2$, (more details will be given for each simulation accordingly). Noting $\mathbf{N}$ and $\mathbf{B}$ the respective interpolation and differentiation matrices, the displacement and damage fields are interpolated as:

$$\begin{aligned} \underline{u}(x) &= \mathbf{N}_u \underline{u}^N \text{ and } \boldsymbol{\varepsilon}(x) = \mathbf{B}_u \underline{u}^N \\ \alpha(x) &= \mathbf{N}_\alpha \alpha^N \text{ and } \nabla \alpha(x) = \mathbf{B}_\alpha \alpha^N \end{aligned} \quad (1.39)$$

where $\underline{u}^N$ and α^N are used to denote the current global displacement and damage nodal vectors.

1.6.2 Explicit time-stepping procedure for the phase-field model

In this section, the above dynamic phase-field model is numerically described. Practically, it consists of solving the elastic-damage dynamic wave equation along with the total energy minimisation. An arbitrary time discretisation (t^n) is considered. The standard Newmark- β integrator is adopted:

$$\dot{\underline{u}}^{n+1} = \dot{\underline{u}}^n + \frac{\Delta t}{2}(\ddot{\underline{u}}^n + \ddot{\underline{u}}^{n+1}) \quad (1.40)$$

$$\underline{u}^{n+1} = \underline{u}^n + \Delta t \dot{\underline{u}}^n + \frac{1-2\beta}{2} \Delta t^2 \ddot{\underline{u}}^n + \beta \Delta t^2 \ddot{\underline{u}}^{n+1} \quad (1.41)$$

The explicit scheme ($\beta = 0$) has been chosen for updating the accelerations, velocities and displacements. The Courant–Friedrichs–Lewy (CFL) time-step is used for the time stepping. The explicit method is preferred mainly in terms of computational efficiency, as it turns out, the time evolution of $(\underline{u}, \alpha)$ is directly decoupled and the two subproblems can be independently solved, comparably to the quasi-static staggered implementation. Details on the implicit and explicit implementations can be found in [Li et al., 2016b]. The following box summarizes the overall algorithm of the explicit time-stepping procedure for the dynamic phase-field model.

Explicit time-stepping procedure for the phase-field model

Initialise $\underline{u}^0$, $\underline{\dot{u}}^0$, α^0 and $\mathcal{H}_c^0 = 0$

Update the damage field α^0 from Equation (1.27)

Initialise the acceleration from Equation (1.26)

while $t^n \leq T$, given $\underline{u}^n$, $\underline{\dot{u}}^n$, α^n , $\mathcal{H}_c^n$ and $\underline{\ddot{u}}^n$

1. Update $\underline{\dot{u}}^{n+1/2} = \underline{\dot{u}}^n + \frac{\Delta t}{2} \underline{\ddot{u}}^n$
2. Update $\underline{u}^{n+1} = \underline{u}^n + \Delta t \underline{\dot{u}}^{n+1/2}$
3. Compute the history function $\mathcal{H}_c^{n+1}$ from Equation (1.21)
4. Compute the damage phase-field α^{n+1} by solving Equation (1.27)
5. Update the internal forces $\underline{F}_{int}(\underline{u}^{n+1}, \alpha^{n+1})$ (following Equation (1.42)) and the acceleration $\underline{\ddot{u}}^{n+1}$
6. Update $\underline{\dot{u}}^{n+1} = \underline{\dot{u}}^{n+1/2} + \frac{\Delta t}{2} \underline{\ddot{u}}^{n+1}$
7. $n = n + 1$ and go to 2

A classical linear FE implementation is considered. The ideal properties of the spatial discretisation are chosen following [Nguyen et al., 2016, Li et al., 2016a]. The mesh size h is usually taken approximately $h \simeq l_c/3$ to $l_c/2$, (more details for each simulation will be given accordingly). The elastic-damage dynamic wave Equation (1.26) becomes:

$$\mathbf{M} \underline{\ddot{u}} = -\underline{F}_{int}(\underline{u}, \alpha) \quad (1.42)$$

where $\mathbf{M}$ denotes the classical consistent lumped mass matrix [Li et al., 2016b] and $\underline{F}_{int}(\underline{u}, \alpha)$ denotes the internal forces vector [Li et al., 2016a]. As mentioned, an explicit

Newmark scheme has been chosen for the update of accelerations, velocities and displacements. Damage irreversibility is ensured as the damage problem is adopted from the quasi-static one. Time steps (temporal discretisation) have been chosen sufficiently small to satisfy the conditional stability of the explicit scheme.

The quasi-static and dynamic phase-field algorithms herein described are implemented using an in-house developed finite element code in MATLAB environment.

Next, an analytical study on the influence of the threshold along with the regularisation parameter.

1.7 Influence of the regularisation parameter l_c

In this section, following [Nguyen et al., 2016, Borden et al., 2012], the influence of the phase-field regularisation parameter l_c is put-forth. The study is extended to the analysis of the elastic threshold ϕ_c coupled with l_c when the former is added to recover an initial elastic phase (Section 1.8). To illustrate these influences, a unidimensional bar under uniaxial tension is first considered (Figure (1.2)). Assuming that Poisson ratio is 0, and with the absence of initial defects, the damage distribution is assumed to be homogeneous, and the non-local part of the crack density function is disregarded $\nabla\alpha = 0$. For uniaxial *monotonic* tension, $\sigma = g(\alpha)\varepsilon E$, the degradation function $g(\alpha) = (1 - \alpha)^2$ is considered. The quadratic crack density function is taken and the initial elastic threshold is disregarded following [Amor et al., 2009, Nguyen et al., 2016]. The irreversibility constraint is imposed by the history function $\mathcal{H}^{t=t_0} = \max(\mathcal{H}^{t<t_0}, W_u^{+,t=t_0})$ with $\mathcal{H}^0 = 0$.

The second part of Equation (1.19) in 1D gives the following energy expression for a homogeneous damage distribution:

$$\begin{aligned} \alpha &= \arg\left\{\inf_{\alpha} \int_{\Omega} \left[g_c \cdot \left(\frac{1}{2l_c} \alpha^2 + \frac{l_c}{2} \nabla \cdot \nabla \alpha \right) + g(\alpha) \mathcal{H} \right] d\Omega \right\} \\ &= \arg\left\{\inf_{\alpha} \left[g_c \frac{1}{2l_c} \alpha^2 + (1 - \alpha)^2 \mathcal{H} \right] \right\} \end{aligned} \quad (1.43)$$

And damage evolution can thus be written as a solution of the minimisation problem (1.43) as:

$$\alpha(\varepsilon) = \frac{2\mathcal{H}}{2\mathcal{H} + \frac{g_c}{l_c}} \quad (1.44)$$

In the case of monotonic loading ($\dot{\varepsilon} \geq 0$) from $\varepsilon^{t=0} = 0$, the constraint of irreversibility on damage can be dropped and $\mathcal{H}$ becomes $\mathcal{H}^{t=t_0} = W_u^{+,t=t_0} = W_u^{t=t_0}$. Damage and stress

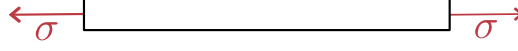


Figure 1.2 – Unidimensional bar under traction for the analysis of the phase-field method parameters in a homogeneous case.

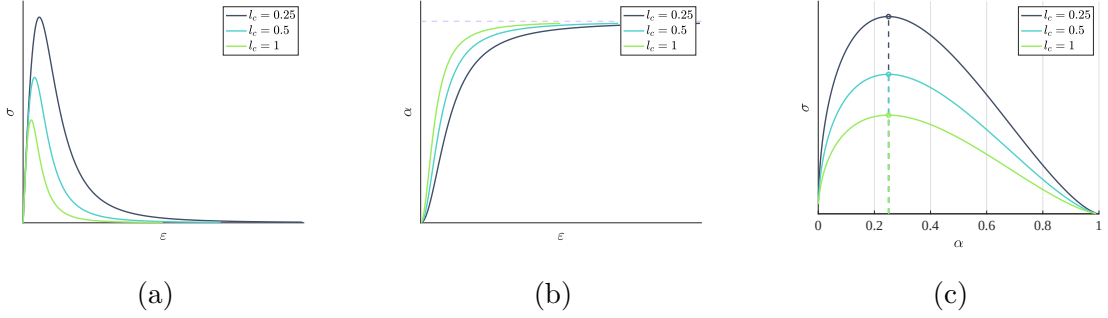


Figure 1.3 – Influence of the regularisation parameter l_c on the homogeneous (stress, strain) (a), (damage, strain) (b) and (stress, damage) (c) relations.

and can be re-written from Equation (1.44) as:

$$\begin{aligned}\alpha(\varepsilon, l_c) &= \frac{\varepsilon^2 E}{\varepsilon^2 E + \frac{g_c}{l_c}} \\ \sigma(\varepsilon, l_c) &= (1 - \alpha)^2 E \varepsilon (l_c)\end{aligned}\tag{1.45}$$

For $E = 1$, $g_c = 1$, the characteristic plots of the (stress, strain) and (damage, strain) relations for different l_c are shown in Figures 1.3(a), (b) and (c). When l_c decreases, the maximum reached stress state (called critical stress σ_c) increases. In fact, by computing the maximum value of the stress with respect to α following:

$$\begin{aligned}\sigma_c &= \max_{\alpha \in [0,1]} \sigma(\alpha(\varepsilon, l_c), l_c), \\ \alpha_c &= \arg\left[\max_{\alpha \in [0,1]} \sigma(\alpha(\varepsilon, l_c), l_c) \right]\end{aligned}\tag{1.46}$$

it's seen that the critical stress state is reached reached at $\alpha_c = 0.25$ (Figure 1.3(c)) independently of l_c and is expressed as $\sigma_c = \frac{9}{16} \sqrt{\frac{E g_c}{3 l_c}}$.

The corresponding evolution of the stress as a function of the damage value is plotted in Figure 1.3(c). It indeed shows that the critical stress is reached at the same damage state $\alpha = 0.25$ independently of l_c . The expressions show that the critical stress will tend to infinity as l_c approaches zero, consistently with Griffith's theory. Note that this relation

only meticulously holds for uniaxial traction without damage gradient and it expresses a unique relation linking the different material properties, which pushed some authors to claim l_c itself as a material parameter, as mentioned previously in Paragraph 1.1. The absence of an initial elastic phase in the stress-strain relation (Figure 1.3(a)), and the initiation of damage at infinitesimal strain-stress levels (Figure 1.3(b)) are noted.

Next, the addition of an elastic threshold onto the strain energy to prevent damage at low stress-strain levels is investigated; and the influence of the arbitrary threshold along the length parameter l_c on the damage-stress-strain relation is put-forth.

1.8 Influence of the elastic threshold ϕ_c

As seen, the absence of an initial elastic phase (quadratic nature of γ) triggers the damage at infinitesimal strains $\varepsilon = \varepsilon_c = 0$. To overcome the absence of an initial elastic threshold, some authors added an artificial initial elastic threshold (e.g., $\phi_c = \frac{g_c}{2l_c}$, [Nguyen et al., 2017]). In this section, we study the influence of an arbitrary threshold $\phi_{c,c}(c) = c\frac{g_c}{l_c}$ on the phenomenological behaviour law of the phase-field model, where the coefficient c is varied between 0, i.e., no threshold and 1. It's noted that the classical $\phi_{c,c}(c) = \phi_c$ occurs at $c = \frac{1}{2}$.

Equivalently to the previous subsection, a bar under uniaxial *monotonic* tension is considered. Poisson ratio is 0, the damage distribution is assumed to be homogeneous. $\sigma = g(\alpha)\varepsilon E$, the degradation function $g(\alpha) = (1-\alpha)^2$ is considered. The quadratic crack density function is taken, and an arbitrary threshold $\phi_{c,c}(c) = c\frac{g_c}{l_c}$ is considered. The irreversibility constraint is imposed by the modified history function $\mathcal{H}_c^{t=t_0} = \max(\mathcal{H}_c^{t<t_0}, W_u^{+,t=t_0} - \phi_{c,c})$ with $\mathcal{H}_c^0 = 0$. Equivalently: The second part of Equation (1.19) in 1D gives the following energy expression for a homogeneous damage distribution:

$$\begin{aligned} \alpha &= \arg\{\inf_{\alpha} \int_{\Omega} [g_c \cdot (\frac{1}{2l_c} \alpha^2 + \frac{l}{2} \nabla \cdot \nabla \alpha) + g(\alpha) \mathcal{H}_c] d\Omega + \phi_{c,c}\} \\ &= \arg\{\inf_{\alpha} [g_c \frac{1}{2l_c} \alpha^2 + (1-\alpha)^2 \mathcal{H}_c] + \phi_{c,c}\} \end{aligned} \quad (1.47)$$

and damage evolution can thus be written as a solution of the minimisation problem (1.47) as:

$$\alpha(\varepsilon) = \frac{2\mathcal{H}_c}{2\mathcal{H}_c + \frac{g_c}{l_c}} \quad (1.48)$$

with $\mathcal{H}_c^{t=t_0} = \max(\mathcal{H}_c^{t<t_0}, W_u^{+,t=t_0} - \phi_{c,c})$ with $\mathcal{H}_c^0 = 0$.

In the case of monotonic loading ($\dot{\varepsilon} \geq 0$) from $\varepsilon^{t=0} = 0$, damage and stress can be re-written from Equation (1.48) as:

$$\alpha(\varepsilon, l_c) = \begin{cases} \frac{\varepsilon^2 E - \phi_{c,c}}{\varepsilon^2 E - \phi_{c,c} + \frac{g_c}{l_c}} & \text{if } \varepsilon \geq \sqrt{\frac{\phi_{c,c}}{E}} \\ 0 & \text{else} \end{cases} \quad (1.49)$$

$$\sigma(\varepsilon, l_c) = (1 - \alpha)^2 E \varepsilon(l_c)$$

And to find the critical stress, Equation (1.46) is re-written to take the threshold into account as:

$$\begin{aligned} \sigma_c &= \max_{\alpha \in [0,1]} \sigma(\alpha(\varepsilon, l_c, c), l_c, c) \\ \alpha_c &= \arg[\max_{\alpha \in [0,1]} \sigma(\alpha(\varepsilon, l_c, c), l_c, c)] \end{aligned} \quad (1.50)$$

which yields the following expression of the critical damage α_c , or the damage at which the critical stress σ_c is reached as a function of the threshold coefficient c :

$$\alpha_c = \frac{8c - 1}{8c - 4} \quad (1.51)$$

And the critical stress σ_c can be written as:

$$\sigma_c = \sigma\left(\frac{8c - 1}{8c - 4}, l_c, c\right) \quad (1.52)$$

Only for the admissible $0 \leq \alpha \leq 1$, with $0 \leq c \leq 1/8$. For $c \geq 1/8$, the maximum stress state is obtained at $\alpha = 0$. For $c = 0$, the standard phenomenological relations (Figure 1.2) are recovered.

Figure 1.4 shows the influence of the threshold coefficient c on the stress-strain-damage behaviour for fixed l_c , $E = 1$ and $g_c = 1$. The presence of the elastic phase at the beginning of the loading of the bar is noted for $c > 0$ (Figure 1.4(a)). When increasing the threshold coefficient c , the critical stress σ_c increases. Moreover, it's obvious how the presence of a threshold is reflected on the phenomenological behaviour: a more brittle response is observed at larger threshold coefficients (Figure 1.4(a)) where the softening phase is much steeper. As mentioned, the problem of damage occurring at low stress-strain levels was prevented, and the critical strain (ε_c at which the damage is initiated) is no longer

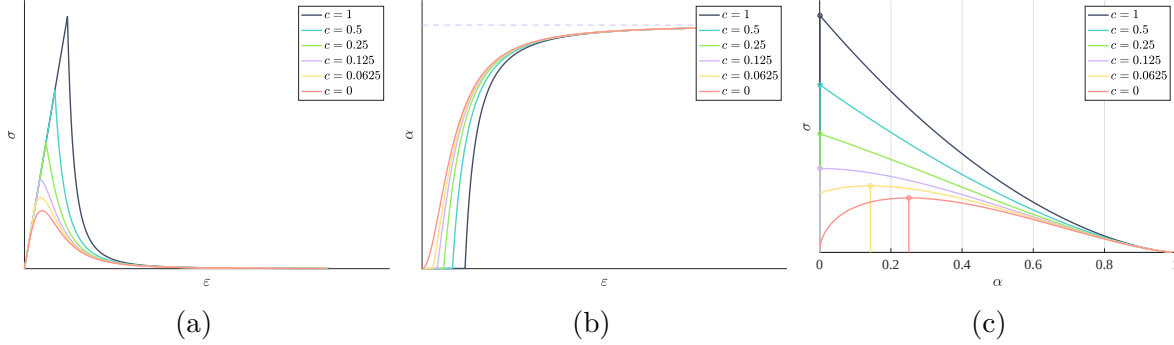


Figure 1.4 – Influence of the threshold coefficient c on the homogeneous (stress, strain) (a), (damage, strain) (b) and (stress, damage) (c) relations.

infinitesimal (Figure 1.4(b)). The corresponding evolution of the stress as a function of the damage value is plotted in Figure 1.4(c). It shows that the critical stress is reached at different damage states for each threshold, and for $c \geq 1/8$, the critical stress is reached at $\alpha_c = 0$ suggesting thus an elastic brittle behaviour until fracture - as opposed to the case where $\alpha_c \neq 0$ and where the critical stress is reached after some degradation of the elasticity, e.g., at $\alpha_c = 0.25$.

A more detailed study on the influence of the threshold on the critical stress and the damage state at which the critical stress is reached is lead. For $0 \leq c \leq 1$, the evolution of the stress σ as a function of the damage state α (Equation (1.50)) is shown in Figure 1.5(a). The critical stress for each threshold coefficient is drawn in 'bittersweet' colour, and the evolution of σ as a function of α at for specific thresholds ($c = 0, 1/16, 1/8, 1/4, 1/2, 1$) are shown. Figure 1.5(c) shows the α_c at which the critical stress σ_c is reached for $0 \leq c \leq 1$. For $c \geq \frac{1}{8}$, it can be seen that the critical stress is always reached in the sound material (in the linear elastic phase (Figure 1.5(c)) suggesting thus that the material behaviour is actually elastic up until failure, a feature that is lost if no threshold is considered.

Additionally, the critical stress (Equation (1.51)) is no longer unique for a set of material parameters ($E = 1, g_c = 1$) and a specific l_c (Figure 1.5(c) shows the evolution of σ_c for fixed E ; g_c and l_c) making the internal length l_c of the phase-field model a numerical parameter corresponding solely to the regularisation of the crack.

Moreover, the ability to manipulate the threshold $\phi_{c,c}$ to simulate more or less brittle materials is obvious. And that without additional costs on the phase-field problem, i.e., without considering perpetually smaller l_c and thus finer finite element meshes h to converge to the brittle failure.

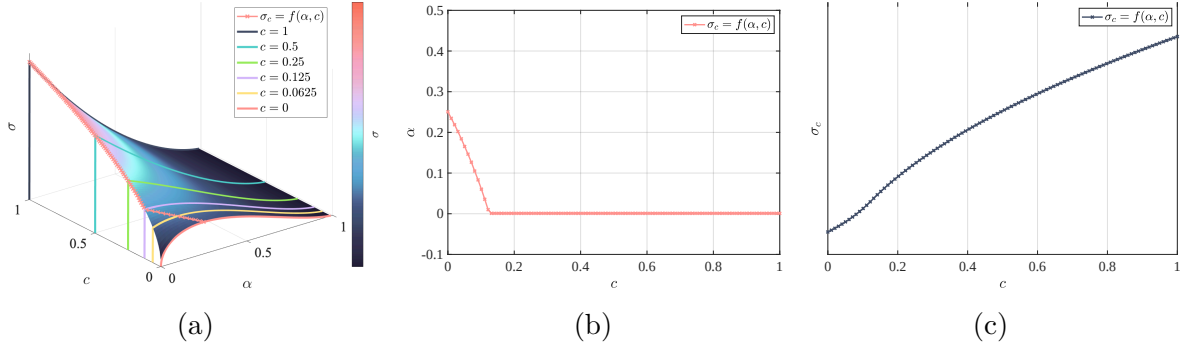


Figure 1.5 – Influence of the threshold coefficient c on the (stress-damage) relation, (a), the damage state α at which the critical stress occurs (α_c) for different threshold coefficients c (b), and the evolution of the critical stress σ_c as a function of the threshold coefficient c (c)

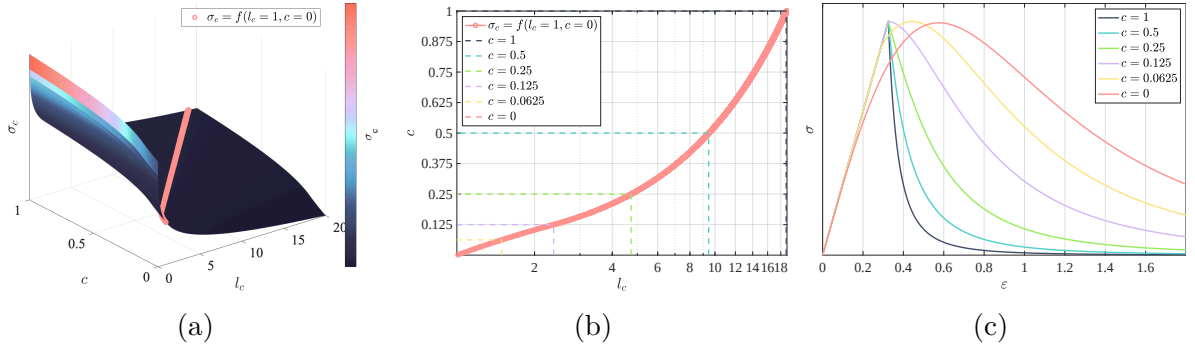


Figure 1.6 – iso- σ_c for different couples of (l_c, c) at fixed g_c . Evolution of σ_c as a function of l_c and c (a), the couples (l_c, c) that yield the same σ_c at fixed g_c (b) and the influence of c on the phenomenological stress-strain relation at fixed (g_c, σ_c) (c)

To illustrate this concept, the critical stress σ_c is computed for $0 \leq l_c \leq 20$ and $0 \leq c \leq 1$ and plotted in Figure 1.6(a) for fixed $E = 1$ and $g_c = 1$. Clearly, different (l_c, c) couples that yield the same critical stress can be found (bittersweet colour which is the intersection of the $\sigma_c = \sigma_c(l_c = 1, c = 0)$ with the surface $\sigma_c(l_c, c)$). Figure 1.6(b) plots the (l_c, c) couples yielding equivalent critical stresses for fixed $g_c = 1$ and $E = 1$. Of course, the actual stress-strain relation would differ and it translates into a more brittle behaviour one as the value of the considered threshold is increased (Figure 1.6(c)). The ability to simulate more or less brittle material behaviours, and to independently choose σ_c and l_c provides the phase-field model with even more adaptability for advanced simulations without adding in complexity.

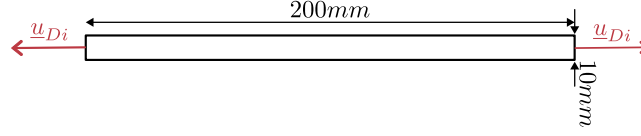


Figure 1.7 – Unidimensional bar under traction for the quasi-static benchmark to validate the implementation and analyse the influence of l_c and c

1.9 Numerical examples

To validate the phase-field and check the length scale sensitivity with the influence of the threshold, a quasi-static uniaxial traction problem with no singularity is considered [Pham et al., 2011a, Linse et al., 2017, Wu and Nguyen, 2018, Mandal et al., 2019a]. The validation in dynamics is carried-out on the standard dynamic crack branching test [Borden et al., 2012, Molnár et al., 2020b].

The goal is to study the influence of the different phase-field parameters on the (i) regularised crack topology and the structural response (ii) in quasi-statics; branching and crack tip speeds in dynamics (iii).

1.9.1 Quasi-static benchmark : Uniaxial traction bar

The quasi-static benchmark present in [Wu and Nguyen, 2018] is investigated. A bar of length $L = 200mm$, of height $h = 10mm$ and unit cross-section under uniaxial traction is considered Figure 1.7; the left and right edges are stretched by a monotonically increasing displacement. The following material properties from the literature are assumed; a Young's modulus $E = 31.25GPa$, Poisson ratio $\nu = 0.25$ and $g_c = 8J/m^2$.

Plane strain conditions are assumed. In the numerical simulations, three length scales $l_c = 5, 10$ and $15mm$ are studied. The mesh size $\frac{h}{\min l_c} = 10$ is taken such as mesh-convergent solutions are guaranteed for all l_c [Nguyen et al., 2016, Mandal et al., 2019a, Linse et al., 2017].

Theoretically, if no imperfections are introduced, the strain and stress fields are strictly uniform in the bar and it's impossible to trigger a local damaging band. However, due to numerical errors / mesh bias, the strain / stress fields are non-uniform allowing thus the trigger of damage [Wu and Nguyen, 2018]. To overcome crack topology errors coming from enforcing the irreversibility via the history field $\mathcal{H}_c^{t=t_0} = \max(\mathcal{H}_c^{t< t_0}, W_u^{+, t=t_0} - \phi_{c,c})$, $\mathcal{H}_c$ here is not treated as a history function but instead as $\mathcal{H}_c^{t=t_0} = W_u^{+, t=t_0} - \phi_{c,c}$ [Linse

et al., 2017].

As shown in [Wu and Nguyen, 2018, Mandal et al., 2019b], the damage band may occur on either edges of the bar. To avoid such a case, a Dirichlet condition $\alpha = 0$ is imposed on both left and right edges of the bar such that the localisation bands can form in the interior of the bars as shown in Figure 1.8.

Multiple combinations of length-scales l_c and threshold coefficients c are considered and are shown in Figure 1.8. As expected, the crack bandwidth broadens as the length scale parameter l_c increases; however, no apparent effect from the threshold on the crack band is observed (observation in Figure 1.9(b) where the damage profiles of the different l_c, c couples are superposed). To quantify the influence of $\phi_{c,c}$ on the crack topology, the evolution of the numerically calculated crack surface Γ_{l_c} (Equation (1.2)) is compared it to its theoretical value Γ (assuming that the final crack surface $\Gamma = h = 10mm$, per unit thickness). It's mentioned that the considered mesh leads to around 1 – 3% numerical errors [Linse et al., 2017, Mandal et al., 2019a]. The following metric is taken to define the error between the theoretical and numerical crack surface:

$$\epsilon_{\Gamma_{l_c}} = \frac{|\Gamma_{l_c} - \Gamma|}{\Gamma} \quad (1.53)$$

Figure 1.9(c) shows the errors $\epsilon_{\Gamma_{l_c}}$ for the three considered length scales with the three threshold coefficients. The errors are more pronounced at the smaller l_c , and it can be explained by the discretisation. For the larger $l_c = 10$ and $15mm$, it's clear that when no threshold is considered, the error drops below 2%, and when considering a threshold, this error increases to around 4% for both cases. It's recalled that the errors on the crack topology coming from the imposed irreversibility via the history field $\mathcal{H}$ are significantly larger than the values obtained here [Linse et al., 2017]. As opposed to the length-scale l_c , even though the threshold $\phi_{c,c}$ was shown to play a major role in the 'brittle' nature of the behaviour, no impact from the threshold on the width of the smeared crack is observed.

Figure 1.9(a) shows the load-displacement curves of those simulations. Unsurprisingly, even for a sufficiently fine mesh, the numerical results are highly dependent on the length l_c , confirming the analytical results presented previously and coherently with literature findings. The addition of an elastic threshold influences the load-displacement curves. In fact, when no threshold is considered, the triggering of damage at infinitesimal strains occurs, which translates to the absence of a linear phase in the displacement-load curve. As the threshold prohibits the damaging at low strains, the elastic phase prior to damaging is

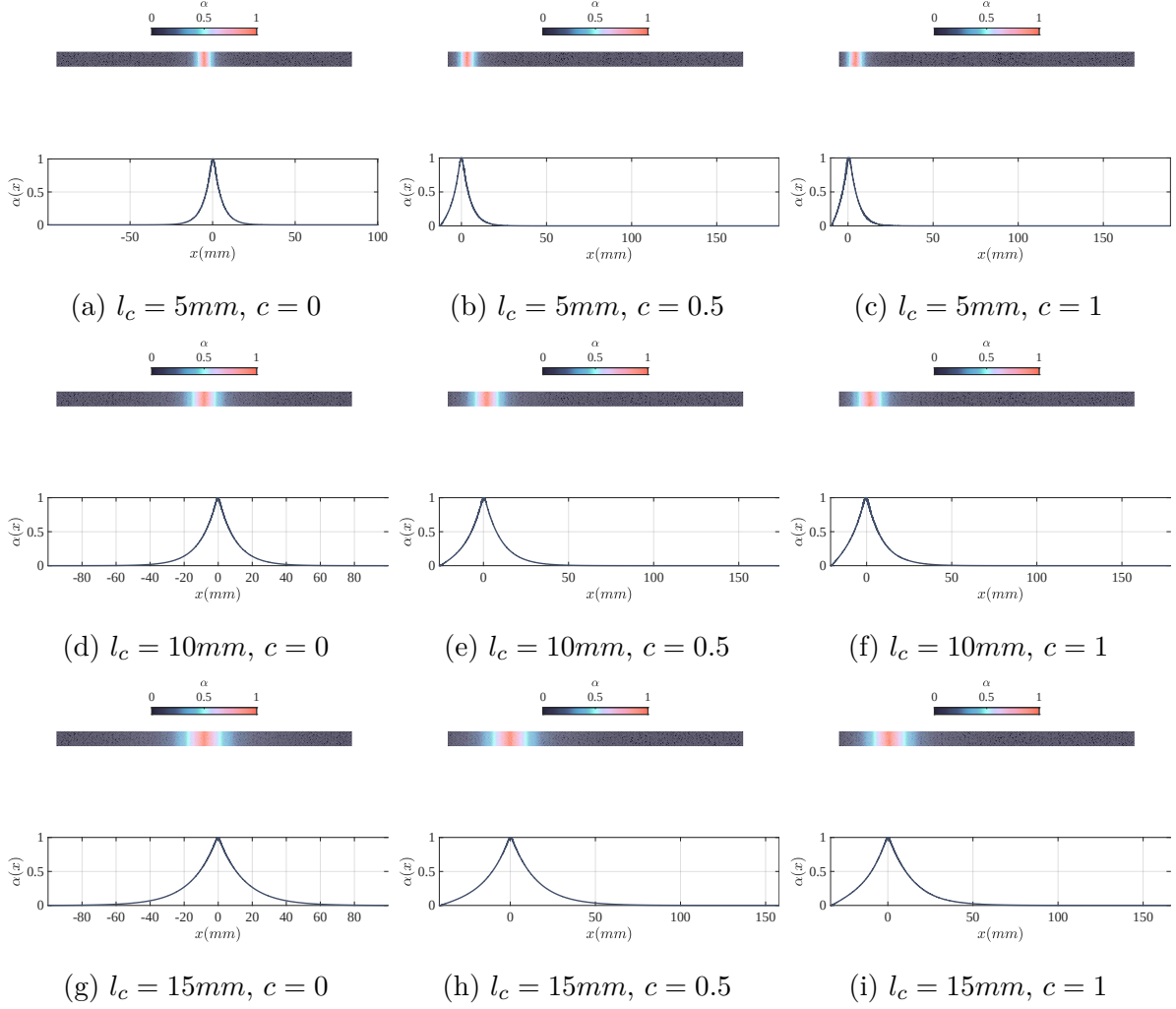


Figure 1.8 – Damage profiles for different length-scales l_c and threshold coefficients.

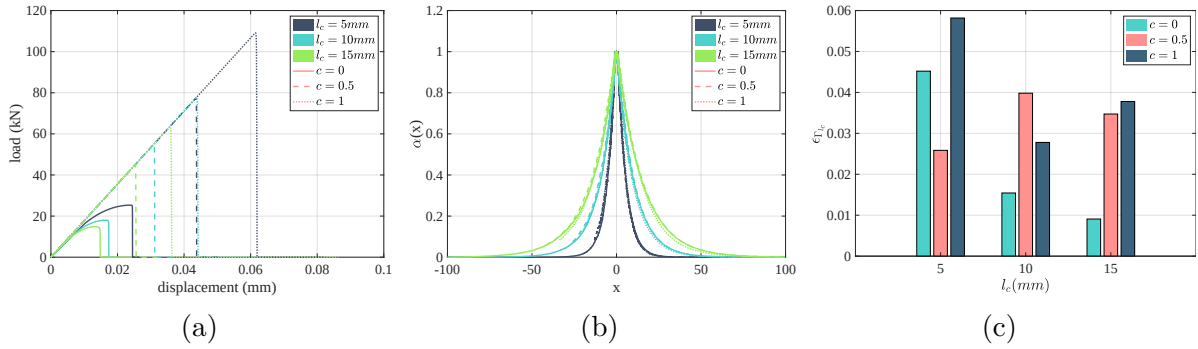


Figure 1.9 – The influence of the threshold and length-scale on the load-displacement curves (a), phase-field profiles (b) and on the crack topology error (c)

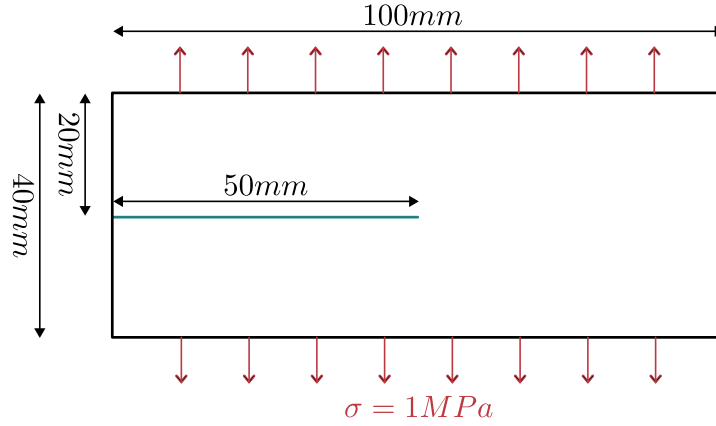


Figure 1.10 – Geometry and boundary conditions for the crack branching benchmark [Borden et al., 2012]

reflected on the load-displacement curves.

The proposed parametrisation of the threshold $\phi_{c,c}$ is thus a robust concept that can be simply implemented to simulate more or less brittle material without diverging from the phase-field theoretical aspect.

After validating the quasi-static phase-field implementation on a simple benchmark, the dynamic implementation is validated on the example proposed by [Borden et al., 2012]. Only the influence of the parametrisation of the threshold $\phi_{c,c}$ is investigated in the next section.⁴

1.9.2 Dynamic benchmark : dynamic crack branching

To determine the effect of the threshold on the *dynamic* crack propagation patterns, and crack tip speeds⁵, and to validate our explicit dynamics implementation, the benchmark example proposed by [Borden et al., 2012] is considered⁴. It's a pre-notched rectangular plate loaded dynamically in tension. The geometry and boundary conditions of the problem are shown in Figure 1.10.

A constant traction load is applied on the top and bottom boundaries of the specimen. The other boundaries are free. The following material properties from [Borden et al.,

4. For a more detailed analysis on the influence of l_c , g_c , and $\phi_{c,c}$ on the dynamic crack patterns, interested readers are referred to Appendix A

5. We developed an algorithm that directly computes the crack tip positions and speeds for multiple cracks in any direction. Interested readers are referred to Appendix B for an schematic representation of the algorithm

2012] are assumed; a Young's modulus $E = 32GPa$ and Poisson ratio $\nu = 0.2$, the length parameter is set to $l_c = 0.25mm$. $g_c = 3J/m^2$. Plane strain conditions are assumed. Three threshold coefficients $c = 0$ ([Borden et al., 2012]), 0.25 and 0.5 are compared.

The crack evolution process in this benchmark example is as follows: the crack initiates from the notch tip and propagates towards the right boundary of the sample. Branching occurs midway Figure 1.11(a).

The fracture patterns are compared to ones obtained in [Borden et al., 2012]. When no elastic threshold is considered, i.e., $\phi_{c,c} = 0$ (Figure 1.11(a), (d)), the patterns are in agreement. The crack initiates at around $12\mu s$ and branches at $48\mu s$. The branching occurs at $79mm$ from the left side of the specimen.

When considering an elastic threshold, and since the material becomes more resistant, the crack path history is modified;

- for $\phi_{c,c} = 0.25\frac{g_c}{l_c}$ (Figure 1.11(b), (d)), a small modification is observed: the crack starts to propagate with a delay of a $3\mu s$ margin (as compared to [Borden et al., 2012]) and branching occurs at $52\mu s$ instead of $48\mu s$. The crack speed trends 1.11(d) are similar, however slightly lower than [Borden et al., 2012]'s, making the branching at $77mm$ instead of $79mm$.
- for $\phi_{c,c} = 0.5\frac{g_c}{l_c}$ (Figure 1.11(c), (d)), the influence of the elastic threshold is more prominent. The initiation is delayed by around $10\mu s$ as compared to [Borden et al., 2012]. The crack speed reaches lower levels (before $t \simeq 50\mu s$). As the material's resistance is increased, the energy provided by loaded boundaries [Broberg, 1996, Broberg, 1964] is insufficient to create new crack faces as fast as in the previous cases leading to slower crack propagation. At $t \simeq 50\mu s$, even though the crack tip speed is comparable to the ones found previously ($c = 0$ and $c = 0.25$), the crack deflects from its original direction of propagation and the emerged branch is directly arrested. This can also be explained by the higher resistance of the material due to the addition of the elastic threshold.

As seen, the addition of a threshold on this benchmark influences both the crack paths and their tip speeds. By making the material more resistant, $\phi_{c,c}$ slightly slows down the crack⁶; plus, by further increasing the threshold, the second branch is rapidly arrested leaving the material with a single crack propagating at slightly higher speeds (as compared to the case where $\phi_{c,c} = 0$, and $0.25\frac{g_c}{l_c}$).

6. The addition of an elastic threshold however does not reduce the maximum reached crack tip speed

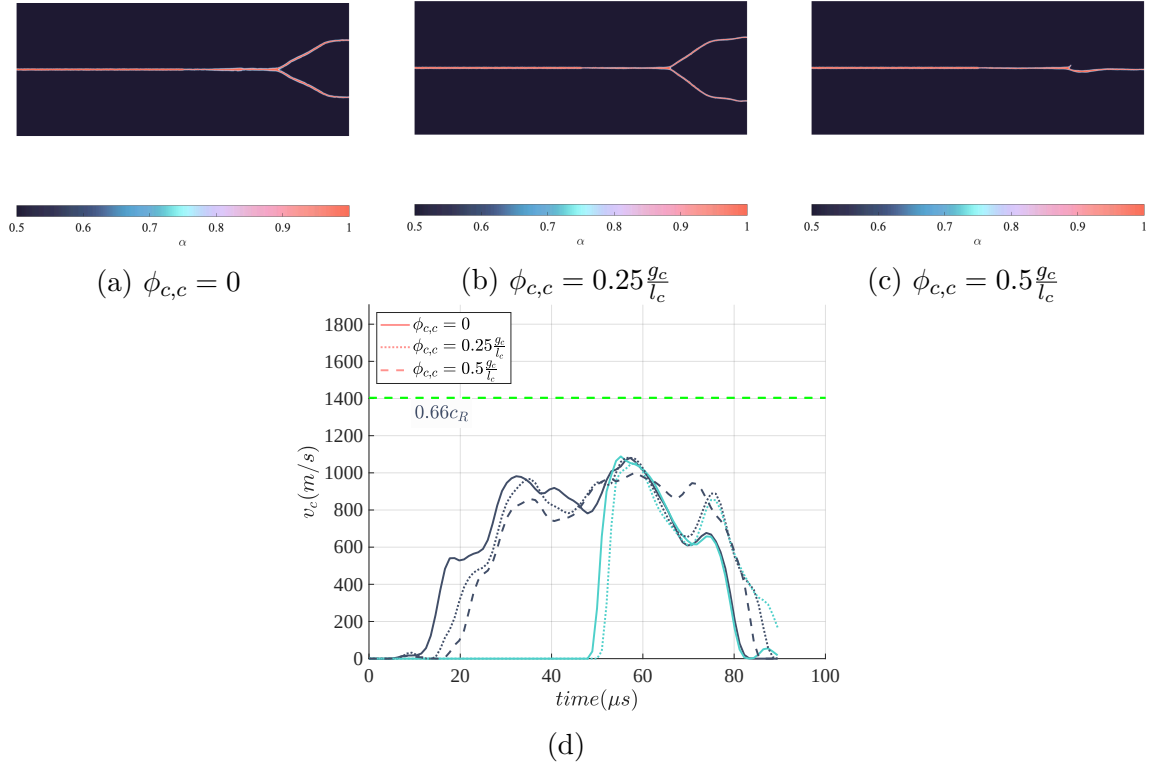


Figure 1.11 – Fracture patterns and crack tip speeds for different elastic thresholds $\phi_{c,c}$. Comparison with the work of [Borden et al., 2012] (no threshold)

Remark 1.2. For interested readers, Appendix A presents further examples showcasing the influence of the phase-field parameters on the crack paths and crack tip speeds on this benchmark (l_c , g_c , fixed g_c/l_c , fixed resistance σ_c by manipulating l_c and $\phi_{c,c}$).

Remark 1.3. In Chapter 5, this benchmark example is re-investigated to analyse the various mechanisms governing the branching phenomena as a result of dynamic instabilities. The influence of the instantaneous crack tip speed coupled with the presence of a stress along the direction of crack propagation on the crack (in)stability is put-forth. Insights on the damage band thickening are advanced. It's noted that the analysis in Chapter 5 is restricted to the crack propagation until branching, hence the rapid crack arrest after branching, i.e., for example in (Figure 1.11(c)) will not be investigated by then.

1.10 Concluding remarks

In this chapter, we reviewed the phase-field method within its computational framework. We showcased its quasi-static and dynamic implementations.

Details regarding the regularisation, the crack density function, the strain energy decomposition, and the history function are given. The overall algorithms for both the dynamic and quasi-static implementations are put-forward.

We validated our implementation on a unidimensional bar in traction and a dynamic crack branching problem.

By parametrising the elastic threshold considered for the quadratic crack density function, we introduced the following contribution to the already robust framework:

- (i) the ability to adjust the critical stress σ_c independently from g_c by considering l_c as a modelling parameter (length scale, regularisation parameter) and not a material parameter. The need for decoupling the toughness g_c , the critical stress (equivalently the strength) σ_c and the length scale parameter is to be put-forth in Chapter 3, where we'll see how in case of microscopically heterogeneous materials, the uniqueness of the relationship of the effective medium between a length-scale, strength and toughness is lost;
- (ii) the ability to perform simulations on a wider range of more or less brittle materials by solely manipulating the threshold $\phi_{c,c}$, i.e., having elastic behaviour until softening (without primarily hardening), having different hardening behaviours;
- (iii) the ability to perform lighter computations, i.e., for fixed g_c and σ_c ; different couples of $(l_c, \phi_{c,c})$ can be interplayed to perform simulations, with the ability to always increase l_c and hence reduce mesh size and computational costs by increasing g_c , of course the influence on phenomenological (stress-strain) behaviour should be kept in mind (regarding the drift towards a more brittle or quasi-brittle behaviour);
- (iv) the recovery of the theoretical crack topology.

All this is believed to allow the phase-field even more adaptability for advanced simulations without adding to its implementation complexity.

This approach is implemented to simulate the failure of the architected materials, and the results would be upscaled via the coarse-graining technique that is covered in the next Chapter 2.

COARSE-GRAINING: FROM MICROSCOPIC TO MESOSCOPIC SCALE(S)

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2.1 Introduction

The global response of a material is often governed by its behaviour at the smaller length scales, e.g., in materials science, the elastic behaviour is influenced by the atomic-lattices reshaping and resizing in metals, or polymer chains stretching in rubbers/polymers; strength, toughness and ductility, are influenced by defects at the microscopic scale; in geotechnics, the permeability of unsaturated soils is influenced by their grain-size distribution. Predicting the macroscopic behaviour of materials from the mechanics of their microstructure has been a subject of intensive research.

A variety of upscaling methods were proposed to reveal the relations between the microstructures from one side and the behaviour at higher scales from the other [Ongaro, 2018]. Aside from determining the effective material properties, there's a relevant need for incorporating small-scale mechanisms of deformation and damage to essentially assess reliability and lifetime of microscopically heterogeneous structures within reasonable computations.

Accordingly, the coarse-graining technique from [Goldhirsch and Goldenberg, 2002]'s work in Molecular Dynamics is adapted to evaluate continuum mechanics at different intermediate mesoscales solely from the gathered data at the microscopic scale and by a manipulation of the inviolable conservation laws. The effective fields of mechanical properties are thus established.

This method allows the construction of consistent density, displacement, strain and stress fields at larger scales based on the actual physics in question at the scale of the heterogeneities. Without any *a priori* on the material's behaviour, the herein proposed scheme provides a genuine evaluation of the effective material and failure properties at the considered scales.

The overview of this chapter is as follows: first, we recall the multiple scales of interest for a failure problem of heterogeneous materials. In Section 2.3, the underlying principles of the coarse-graining method are showcased, the method's parameters and briefly discussed. A continuum mechanics adaptation of the coarse-graining method as seen in [Goldhirsch and Goldenberg, 2002] is followed in Sections 2.4 and 2.5, and a general application scheme is forwarded. Finally, two numerical examples are considered (Section 2.6) to validate the proposed approach: (i) an analysis of a Periodic lattice of holes, for which the coarse-grained mechanical properties (density and elasticity) can be compared to the standard *RVE*-based homogenisation methods. And (ii) an application on analytical solutions for

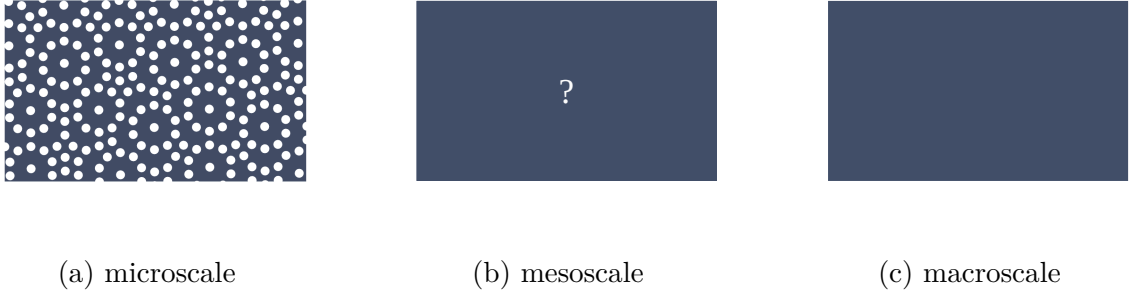


Figure 2.1 – The scales of interest for the failure problem of microscopically heterogeneous materials: the microscopic scale (a) the intermediate mesoscopic scale(s) with properties obtained upon the length scales considered (b) and the structural macroscopic scale (c).

the displacement and stress fields around a crack that validates the applicability of the coarse-graining technique when sharp localisation, i.e., crack, exists.

2.2 Scales of interest

We start this chapter by briefly recalling the multiple scales of interest at which damage problems can be tackled: the microscopic level, the macroscopic level and the mesoscopic level(s) in between:

- The microscopic level is the level at which the material’s architecture is prominent. Continuum mechanics apply; brittle failure occurs and can be simulated by the linear elastic fracture mechanics or its approximations (Phase-field Modelling [Francfort, 1998], Eigen erosion [Pandolfi and Ortiz, 2012]...).
- At the macroscale, the material is seen as a homogeneous bulk (Figure 2.1(c)), where linear elastic fracture mechanics elements can be implemented, and microstructural features give rise to resistance-curve behaviour. Effective macroscopic physical parameters shall be determined.

In between those scales are the mesoscales.

- At the mesoscales, the literature suggests considering a homogeneous material (Figure 2.1(b)), and the effects of the microstructural heterogeneities are implemented in the modelling with the introduction of a process zone of size related to a certain length parameter to which damage spreads. Phase-Field Modelling, Eigen Erosion

and Thick Level Set applied to quasi-brittle failure are examples of models considered at this scale.

The homogeneity of the fields at the intermediate mesoscales is put into question in this study and the *bottom-up* approach is considered to answer the arisen questions.

2.3 Coarse-graining technique principles

The goal of the coarse graining is to produce continuum equations out of information from the smaller scales. When seeking to find continuum mechanics for the fracture process, out of information gathered at the microscopic scale, the challenge is to find an appropriate technique that takes into consideration the real solicitation of the material as well as the singularities coming from crack propagation and the presence of the heterogeneities. The micromechanical fields (that can be generated from phase-field simulations, or from analytical solution, or experimentally gathered, etc.) are upscaled by adapting the method from [Goldhirsch and Goldenberg, 2002]’s work in Molecular Dynamics: a physically consistent upscaling coarse-graining method that allows going from discrete probability density into an upscaled continuum (Figure 2.2).

The parameters of this method are:

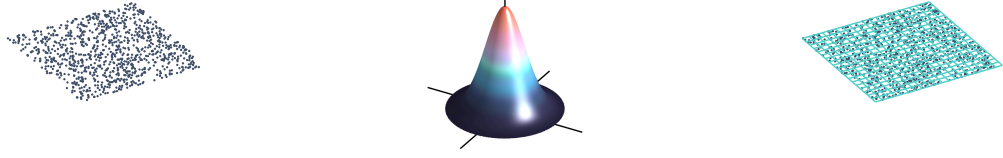
- the convolution or the coarse-graining function ϕ that can be any sufficiently regular function with a local support: a variety of forms were studied and similar results were obtained; in this work, the normalised Gaussian distribution (Figure 2.2(b)) of zero mean μ and a standard deviation σ is considered. It takes the following form:

$$\phi(x, \sigma, \mu) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2(\sigma)^2}} \quad (2.1)$$

- the width of the convolution function $l_{CG} = w/2$. In Equation 2.1, $w = 2 \times 3\sigma$: it’s the most important parameter that defines the different length-scales at which the problem is inspected. The normalised Gaussian function can be rewritten as follows:

$$\phi_{l_{CG}}(x, l_{CG}) = \frac{1}{\frac{l_{CG}}{3}\sqrt{2\pi}} e^{-\frac{x^2}{2(\frac{l_{CG}}{3})^2}} \quad (2.2)$$

- the discretisation H considered for the coarser mesh (the support for the coarse-graining): this parameter defines the resolution of the coarse-grained fields (Figure



(a) Random particle system (b) Gaussian Distribution (c) Mesh support

Figure 2.2 – The coarse-graining function (b) sweeps over the different points in the domain (c), Information from the particles system (a) is smoothed and continuous fields are computed

2.2(c)) and does not affect their distribution. Identical results are obtained from investigations on multiple discretisation sizes validating thus the mesh objectivity of the proposed upscaling technique.

In [Goldhirsch and Goldenberg, 2002], a system of particles indexed by e is considered (Figure 2.2(a)), with known masses $m_e(t)$ and centres of masses $\underline{r}_e(t)$ at time t . The coarse-grained mass density at position r and time t is given by:

$$\rho(\underline{r}, t) \equiv \sum_i m_e \phi[\underline{r} - \underline{r}_e(t)] \quad (2.3)$$

Unlike in [Goldhirsch and Goldenberg, 2002], continuum data is considered at the fine-scale from the micromechanical simulations. Let Ω^0 be the domain of interest in the microstructure, a discretisation of Ω^0 into finite elements serves as a support for the coarse-graining computations. Unlike in [Glasser and Goldhirsch, 2001], here only spatial, and not temporal coarse graining, is invoked. The coarse-grained mass density $R(\underline{x}, t)$ at position $\underline{x}$ in Ω^0 , at time t , is defined as the convolution between the microscopic density function ρ and the predefined coarse-graining function ϕ :

$$R(\underline{x}, t) = \int_{\Omega^0} \rho(\underline{x} - \underline{x}', t) \phi(\underline{x}', t) d\mathbf{x}' \quad (2.4)$$

For the sake of simplicity, the following notation is considered to replace the convolution:

$$\langle \rho(\underline{x}, t) \rangle_\phi = \int_{\Omega^0} \rho(\underline{x} - \underline{x}', t) \phi(\underline{x}', t) d\underline{x}' \quad (2.5)$$

and the coarse-grained mass density $R(\underline{x}, t)$, at position $\underline{x}$ and time t , would be as follows:

$$R(\underline{x}, t) = \langle \rho(\underline{x}, t) \rangle_\phi \quad (2.6)$$

From this spatial/temporal definition of the coarse-grained mass density, and by imposing the mechanical conservation laws at both the microscopic and coarse-grained scale, expressions for the impulsions, velocities, displacements and stresses are obtained at different positions $\underline{x}$ and times t , at the coarse-grained scale. We start by recalling the conservation laws written at the microscopic scale; i and j denote the different directions in the considered space:

— Balance of Mass

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho \dot{u}_i)}{\partial x_i} = 0 \quad (2.7)$$

— Balance of Momentum

$$\frac{\partial}{\partial t} \rho \dot{u}_i + \frac{\partial}{\partial x_i} \rho \dot{u}_i \dot{u}_j = \frac{\partial}{\partial x_j} \sigma_{ij} \quad (2.8)$$

2.4 Balance of mass

A simple manipulation of Equation (2.7) allows the computation of the expression for the velocity at the coarse-grained scale. Computing the convolution of both sides of the equation, one can obtain:

$$\left\langle \frac{\partial \rho}{\partial t} \right\rangle_\phi = - \left\langle \frac{\partial(\rho \dot{u}_i)}{\partial x_i} \right\rangle_\phi \quad (2.9)$$

The left side of the equation denotes the time derivative of the coarse-grained density $R(\underline{x}, t)$:

$$\frac{\partial R}{\partial t} = - \left\langle \frac{\partial}{\partial x_i} \rho \dot{u}_i \right\rangle_\phi \quad (2.10)$$

Using the basic rule of the derivation of convolution, one can write:

$$\frac{\partial R}{\partial t} + \frac{\partial}{\partial x_i} \langle \rho \dot{u}_i \rangle_\phi = 0 \quad (2.11)$$

Writing the balance of mass at the coarse-grained scale, with $R\dot{U}_i$ denoting the impulsion P_i at the coarse-grained scale:

$$\frac{\partial R}{\partial t} + \frac{\partial}{\partial x_i} R\dot{U}_i = 0 \quad (2.12)$$

and by identification between Equation (2.11) and Equation (2.12), we can conclude that

$$R\dot{U}_i = \langle \rho u_i \rangle_\phi \quad (2.13)$$

2.4.1 Coarse-Grained velocity

Identifying the coarse-grained impulsion, $P_i = R\dot{U}_i$, and the microscopic impulsion, $p_i = \rho \dot{u}_i$, one can see that the coarse-grained impulsion is equal to the coarse-graining of the microscopic impulsion, which is not the case for the velocity field. The velocity at the coarse-grained scale is the ratio between the upscaled impulsion and the coarse-graining mass density:

$$\dot{U}_i = \frac{\langle \rho \dot{u}_i \rangle_\phi}{R} = \frac{\langle p_i \rangle_\phi}{R} = \frac{P_i}{R} \quad (2.14)$$

2.4.2 Coarse-Grained displacement

In this study, continuum mechanics is assumed to hold in all length scales involved; the derivation is restricted to small displacement gradients and the discussion is confined to analysis on perfectly solid materials. The displacement U_i can be obtained by integrating the coarse-grained velocity $\dot{U}_i$ over time.

In quasi-static problems, the coarse-grained displacement U_i and velocity $\dot{U}_i$ fields have similar expressions, from Equation (2.14):

$$U_i = \frac{\langle \rho u_i \rangle_\phi}{R} \quad (2.15)$$

2.4.3 Coarse-Grained strain and strain rate

Next, it is natural to proceed with a strain calculation based on the coarse-grained velocities, and displacements:

$$\underline{\underline{E}} = \frac{1}{2}(\underline{\underline{\nabla}}\underline{\underline{U}} + \underline{\underline{\nabla}}^T\underline{\underline{U}}) \quad (2.16)$$

$$\underline{\underline{E}} = \frac{1}{2}(\underline{\underline{\nabla}}\dot{\underline{U}} + \underline{\underline{\nabla}}^T\dot{\underline{U}}) \quad (2.17)$$

2.5 Balance of linear momentum

At the microscopic scale, the balance of linear momentum states:

$$\frac{\partial}{\partial t}\rho\dot{u}_i + \frac{\partial}{\partial x_i}\rho\dot{u}_i u_j = \frac{\partial}{\partial x_i}\sigma_{ij} \quad (2.18)$$

at the mesoscopic scale, a similar expression is expected with coarse-grained mechanical fields, to be written as:

$$\frac{\partial}{\partial t}R\dot{U}_i + \frac{\partial}{\partial x_i}R\dot{U}_i\dot{U}_j = \frac{\partial}{\partial x_i}S_{ij} \quad (2.19)$$

From the time derivative of the coarse-grained impulsion $P_i = R\dot{U}_i = \langle \rho\dot{u}_i \rangle_\phi$ (Equation (2.13)), and using the basic rule of derivation, the expression of the stresses at the coarse-grained scale is determined:

$$\frac{\partial P_i}{\partial t} = \left\langle \frac{\partial}{\partial t}\rho\dot{u}_i \right\rangle_\phi \quad (2.20)$$

from the balance of momentum at the microscopic scale Equation (2.8), we can write Equation (2.20) as:

$$\frac{\partial P_i}{\partial t} = \left\langle \frac{\partial}{\partial x_i}(\sigma_{ij} - \rho\dot{u}_i\dot{u}_j) \right\rangle_\phi \quad (2.21)$$

It's here interesting to introduce what is called 'fluctuating velocity' $\dot{u}_i' = \dot{u}_i - \dot{U}_i$. This velocity does not add any impulsion to the system, and the coarse-grained fluctuation impulsion vanishes as:

$$\langle \rho\dot{u}_i' \rangle_\phi = \int \rho(\dot{u}_i(\underline{x} - \underline{x}', t) - \dot{U}_i(\underline{x}, t))\phi(\underline{x})d\underline{x}' = \langle \rho\dot{u}_i \rangle_\phi - \dot{U}_i\langle \rho \rangle_\phi = P_i - R\dot{U}_i = 0 \quad (2.22)$$

Once, $\dot{u}_i$ is replaced in Equation (2.21) by $\dot{u}_i' + \dot{U}_i$, the following equation can be written:

$$\frac{\partial P_i}{\partial t} + \frac{\partial}{\partial x_i}R\dot{U}_i\dot{U}_j = \frac{\partial}{\partial x_i}\langle \sigma_{ij} - \rho\dot{u}_i'\dot{u}_j' \rangle_\phi \quad (2.23)$$

2.5.1 Coarse-Grained stress

Now writing the coarse-grained balance of linear momentum as a function of the coarse-grained variables, and by identification between Equation (2.23) and (2.19) the

expression of the stress at the coarse-grained scale is obtained:

$$S_{ij} = \langle \sigma_{ij} - \rho \dot{u}_i' \dot{u}_j' \rangle_\phi \quad (2.24)$$

In quasi-statics, the dynamic terms $\dot{u}_i' \dot{u}_j'$ will be neglected and the stress at the coarse-grained stress field $\underline{\underline{S}}$ scale is found to be equivalent to the convolution of the microscopic stress field with the coarse-graining function: $\underline{\underline{S}} = \langle \underline{\underline{\sigma}} \rangle_\phi$.

Finally, from equations Equation (2.15), Equation (2.16) and Equation (2.24), displacement, strain and stress fields are constructed out of micromechanical fields. As seen, this upscaling technique requires no condition on the geometrical aspect of the microstructure, nor on the micromechanical fields, nor puts any *a priori* on the behaviour at the mesoscopic scales. It's indeed applicable on arbitrary heterogeneous (e.g., non-periodic) materials even when sharp localisation is present. The following box summarizes the overall algorithm of the application of the proposed coarse-graining method.

A general scheme of analysis based on the proposed coarse-graining method within the finite element configuration

Acquire the microscopic displacement, stress and strain (numerical simulations, analytical solutions, etc.)

Choose the domain of interest Ω^0 , the coarse-graining support mesh H and the coarse-graining scales l_{CG} _____

Coarse-grain the mechanical fields for each l_{CG}

1. Map microscopic finite elements to their corresponding grain(s), and compute Equation 2.2
2. From the definition of the coarse-grained density, compute R (Equation 2.6)
3. From the balance of mass, compute the coarse-grained velocity field $\underline{V}$ (Equation 2.14) and deduce the coarse-grained displacement field $\underline{U}$
4. From the balance of momentum, compute the coarse-grained stress field $\underline{\underline{S}}$ (Equation 2.24)

Remark 2.1. *The general scheme of analysis is herein presented within the framework of this study (application on mechanical fields coming from simulations), of course it can be adapted to other cases, e.g., the coarse-graining of full-field experimental measurements (digital image correlation DIC) to obtain consistent coarse-grained displacement, strains*

and strain-rates.

Remark 2.2. *It's mentioned that all the computations are made using an in-house MATLAB finite element code.*

<https://github.com/dengwirda/find-poly> provided an efficient grain-element mapping algorithm. (up to 500% efficiency boost as compared to built-in MATLAB function.)

2.6 Numerical examples

In this section, the implementation of the coarse-graining scheme is validated on a Periodic lattice of holes, for which the coarse-grained mechanical properties (density and elasticity) are compared to the standard *RVE*-based homogenisation methods. Of course, the conditions of applicability and validity of the standard homogenisation method are sought for thorough comparison, hence the application on simple Periodic lattice under the condition that no large gradients of deformation nor localisation occur. The second application validates the applicability of the herein proposed coarse-graining technique when sharp localisation, i.e., presence of crack, exists.

2.6.1 Application on a hexagonal distribution of holes

First, a validation on a hexagonal distribution of holes (Figure 2.3(a)) is sought. The microstructure's symmetry order (6) should lead to elastic isotropic equivalent media [Auffray, 2008]. The holes' spacing is of $d = 300\mu m$; they have a radius $r_h = 750\mu m$ leading to a volume fraction of the bulk of 78%. The unit-cell *RVE* is shown in figure 2.3(b). For this application, the following mechanical properties are considered: $E = 3GPa$, $\nu = 0.35$ and $\rho = 1200kg/m^3$. A rectangular architected sample is considered. Within the finite element framework, the specimen is meshed with triangular finite elements of size $h = 20\mu m$. The coarse-graining support domain is put at the core at the specimen and coarser elements $H = 1mm$ are considered (Figure 2.4).

From Equation 2.6, the coarse-grained density field in the support domain can be determined. Figure 2.4 shows the evolution of the density fields $R(\underline{x})$ at three coarse-graining scales $l_{CG}/d = 1/2, 2$ and 4. As the implemented coarse-graining method is based on the inviolable conservation laws - mass continuity between them -, it can be seen that the mean effective density in the studied domain (Figure 2.5) is conserved through the scales and only the homogeneity of the field is altered. The volume fraction (78%) is

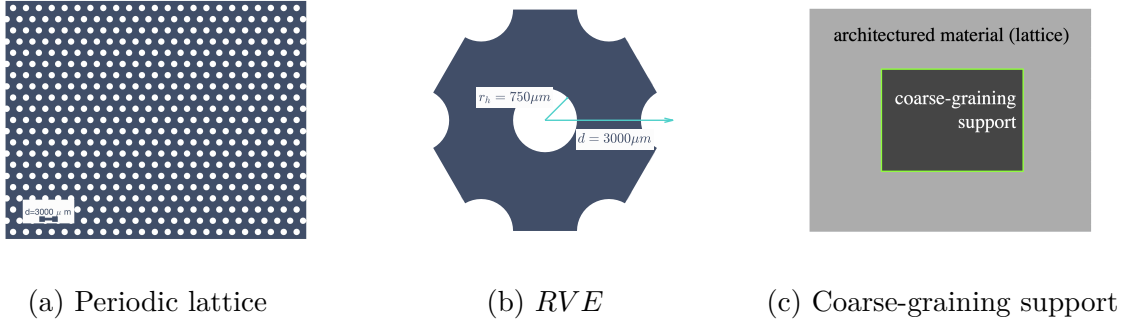


Figure 2.3 – The Periodic lattice (hexagonal distribution) (a) and its one-unit-cell RVE (b). The Periodic lattice and the coarse-graining support Ω_0 (c)

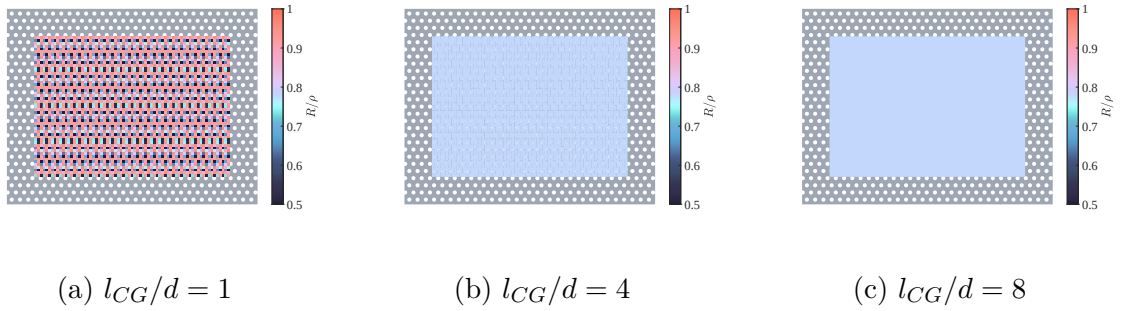


Figure 2.4 – Effective density fields of the Periodic lattice

recovered. It's observed that heterogeneities of the effective density of the material are smeared-out at $l_{CG}/d = 1$. It's considered that the homogeneity of a field is attained once its corresponding coefficient of variation COV drops below the $\leq 1\%$ threshold. The arithmetic mean is calculated as the sum of the sampled values (whether at the nodes or the Gaussian points of the coarse elements in the coarse-graining support domain Ω_0) divided by the total number of samples (nodes and Gaussian points respectively). The standard deviation is found by taking the square root of the average of the squared differences of the values from their mean value. The coefficient of variation is defined as the ratio of the standard deviation to the arithmetic mean. (More details about this 'homogenisation' of the mechanical fields can be found in Chapter 3).

The focus is now turned to the ability of the coarse-graining technique to determine the effective elasticity tensor at the different scales. The obtained elasticity tensor is compared to results coming from the periodic homogenisation technique.

Two tensile and one shear test simulations are conducted on the specimen. From the microscopic mechanical fields, coarse-grained displacements, strains and stresses can be

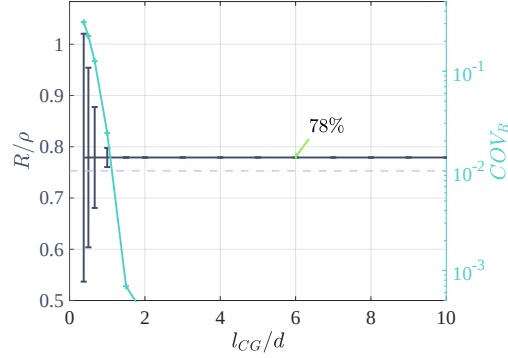


Figure 2.5 – Density conservation through the scales l_{CG} and the evolution of the corresponding coefficient of variation COV_R

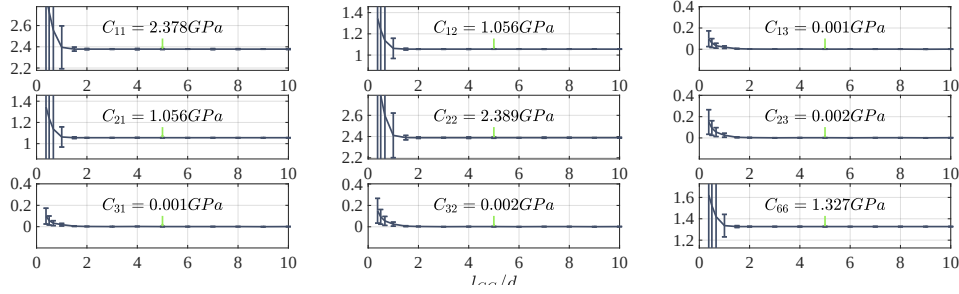


Figure 2.6 – Mean values of the effective stiffness tensor and their deviation at different coarse-graining scales l_{CG}/d (abscissa)

evaluated for different l_{CG} . Coarse-grained strain and stress couples obtained from the three tests, provide an evaluation of the nine components C_{ij} of the stiffness tensor $\mathbb{C}$, representative of the elastic behaviour. The reduced expression for the effective elasticity tensor in 2D is adopted:

$$\begin{bmatrix} S_{11} \\ S_{22} \\ S_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{16} \\ C_{21} & C_{22} & C_{26} \\ C_{61} & C_{62} & C_{66} \end{bmatrix} \begin{bmatrix} E_{11} \\ E_{22} \\ 2E_{12} \end{bmatrix} \quad (2.25)$$

Figure 2.6 shows the evolution of the different components of the stiffness tensor of the material points with the considered coarse-graining scale l_{CG} . The mean values (at each l_{CG}) of the components of the effective stiffness tensor converge towards their long-scale effective limit starting from considerably small scales ($l_{CG}/d \geq 1$, half the size of the unit-cell RVE). Moreover, These results converge rapidly ($l_{CG}/d \geq 1.5$) to the values

obtained from the periodic homogenisation $\mathbb{C}_{P.H.}$ technique applied on the *RVE* with one unit cell (Figure 2.3(b)):

$$[\mathbb{C}_{P.H.}] = \begin{bmatrix} 2.374 & 1.053 & 0 \\ 1.053 & 2.375 & 0 \\ 0 & 0 & 1.321 \end{bmatrix} GPa, \quad (2.26)$$

within a relative mean square error of 0.6%. More details about the parameters considered for this application can be found in Chapter 3 where we detail the influence of the scale on the material behaviour.

As outlined, the coarse-graining implementation was successfully validated on a Periodic lattice of holes, and results are found to be consistent with the standard techniques found in the literature.

Next, the ability of the proposed method to smear-out sharp localisations is put to the test.

2.6.2 Application on asymptotic analytical static fields

To validate the applicability of this method in cases where sharp localisations exist, the coarse-graining scheme is applied on analytical displacement and stress fields around a crack tip. As seen in the introduction, the presence of a crack induces a discontinuity of the mechanical fields. The coarse-graining technique is expected to smear-out the sharp localisation, see e.g., Figure 2.7, that shows a schematic representation of the stress distribution and the displacement jump smoothened by a Gaussian filter, while conserving mass, energy and momentum balance.

A semi-infinite straight crack in a 2D elastic body -of shear modulus μ and Poisson ratio ν - is considered. The expression of the in-plane stresses and in-place displacement fields are given in Chapter 0.

Generation of the analytical fields

The theory of linear elastic fracture mechanics characterises the stress state near the crack front for a linear elastic isotropic material (Chapter 0). The presence of a crack induces a discontinuity of the mechanical fields which is at the origin of the singularity at the crack tip (the stresses tend to infinity). In order to generate the analytical fields on which the coarse-graining technique will be applied, a grid of data points representing

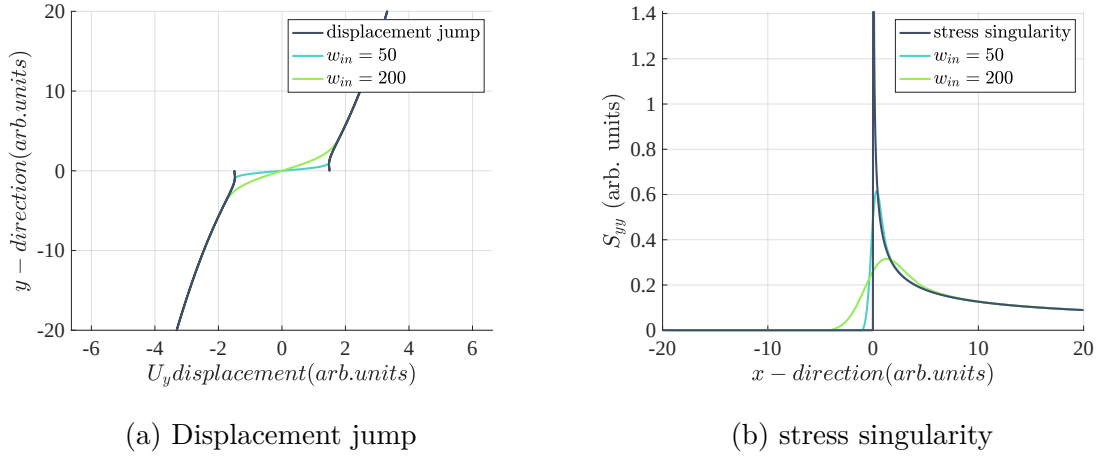


Figure 2.7 – Schematic representation of the problem: the displacement jump and stress singularity and the application of a Gaussian unidimensional filter to the plots

a body is considered. A crack tip is assumed to be propagating horizontally along the middle of the grid at each stepping. For each position of the crack tip, the leading term (K_I) is considered to generate a displacement field in the domain at the vicinity of the crack tip. The ingredients can be summarised as follows:

- Grid data (dimension and size)
- Material elastic properties
- Plane strain / plane stress assumption
- Position of the crack tip
- SIF and higher order terms, i.e., T - stress.

In a 2D elastic body ($\rho = 1200 \text{ kg/m}^3$) of $E = 3 \text{ GPa}$, $\nu = 0.35$ elastic properties, within the plane strain configuration, a horizontal crack travelling in pure mode I at $K_I = 1.5 \text{ MPa}\sqrt{\text{m}}$, yields the displacement fields at the vicinity of the crack tip depicted in Figure 2.8(a). The corresponding stress distribution is shown in Figure 2.8(b). The visualised domain corresponds to the coarse-gaining support domain Ω_0 , i.e., the zone in which the upscaled fields will be computed.

After acquiring the evolution of the stress and displacement fields along the advancement of the horizontal crack inside the domain (left to right), the coarse-graining technique is applied.

Coarse-grained displacement and stress fields

Delaunay triangulation of the discretized data enables the application of the proposed coarse-graining technique. As previously established, the density field is first computed on a coarse-graining support mesh. For this exercise, the coarse mesh size H is set to $H = l_{CG}/5$.

Of course, the density R accross the scales is conserved and is equivalent to $R = \rho = 1200kg/m^3$ (homogeneous body). The analysis is then followed on the displacement fields, strain fields and stress fields. Figure 2.8 shows the upscaled fields at two different coarse-graining scales corresponding to $l_{CG} = 500\mu m$ and $l_{CG} = 1000\mu m$ respectively.

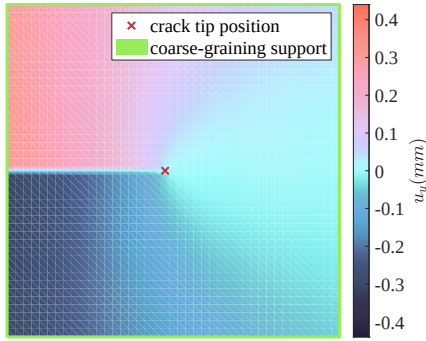
The regularisation of the localisation by the coarse-graining technique is noted. In fact, both the displacement and the stress singularity were regularised. The smoothening of the fields depends directly on the considered coarse-graining scale. In the following Chapter 3, the influence of the coarse-graining scale on heterogeneous materials at different transitional scales (from scale of heterogeneities towards an "effective" representation of the material) is exhibited. An in-depth analysis based on the coarse-graining technique is to be lead.

As seen in this section, displacement and stress fields at the vicinity of a horizontal crack are upscaled; hence, "equivalent" coarse-grained displacements, strains and stresses can be obtained.

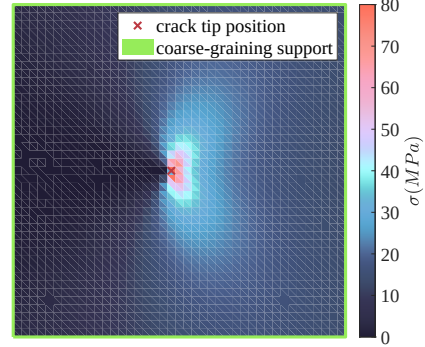
On the coarse-grained stress-strain behaviour

The jump on the crack faces is smoothed as the observation scale (l_{CG}) increases and the sharpness of the crack is smeared-out. Being able to link the *LEFM*, knowingly, the stress and displacement solution to damage mechanics has always been a challenge in the community. With the ability to link discontinuous/singular mechanical fields related to *LEFM*, via the coarse-graining scale, to effective continuous fields; damage mechanics components naturally emerge, and an effective stress-strain relation can be forecasted.

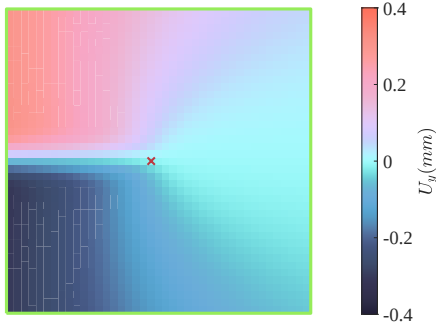
The coarse-grained strains and stresses are confronted. Thanks to the symmetry properties of the considered simple crack-propagation case, the stress-strain history of the different points along a horizontal line are precisely equivalent. The history of the coarse-grained stresses for each point in the coarse-graining support are plotted against their corresponding coarse-grained strains in Figure 2.9 at two l_{CG} . A stress-strain relation at the coarse-graining scale naturally emerges.



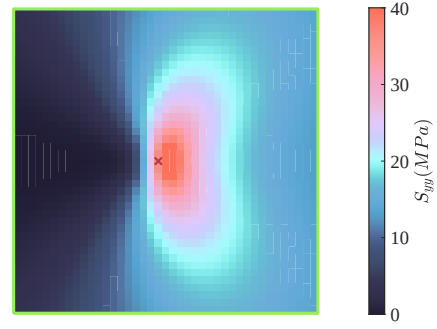
(a) u_y , analytical solution



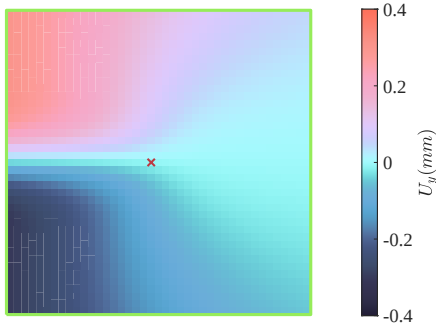
(b) σ_{yy} singularity, analytical solution



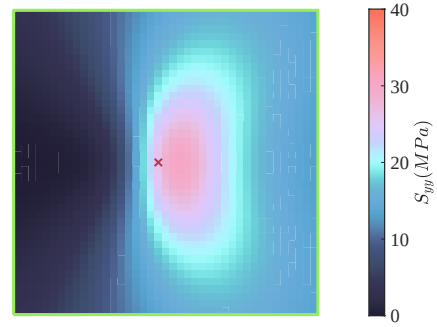
(c) Coarse-grained U_y at $l_{CG} = 500\mu m$



(d) Coarse-grained S_{yy} at $l_{CG} = 500\mu m$



(e) Coarse-grained U_y at $l_{CG} = 1000\mu m$



(f) Coarse-grained S_{yy} at $l_{CG} = 1000\mu m$

Figure 2.8 – Displacement and stress fields at the vicinity of a horizontal crack. The discontinuity of the displacement field and the singularity of the stress field are regularised by the coarse-graining. This regularisation is dictated by l_{CG}

For the two considered length scales, the effective material behaviour appears to undergo a linear elastic trend before its degradation. Non-uniqueness of the stress-strain response is noted when studying the response in a neighbourhood around the crack. The curve reaching the maximum stress corresponds to the response of the points along the crack path. As the distance to the crack path d_c increases, the stress-strain response of the corresponding points reach lower maximum stress states. When the points are much further to the crack path ($d_c > l_{CG}$), they remain undamaged and show typical linear elastic stress-strain response. When observing the behaviour of the data points closest to the crack path, it's obvious how the linear elastic region at the initial states of loading are followed by a non-linear region before reaching the critical stress where softening occurs: this suggests typical *quasi-brittle* effective behaviour. The critical stress σ_f (the maximum stress state reached at the mesoscopic scales from the mesoscopic stress-strain equivalent response) reached at each l_{CG} depends unsurprisingly on the considered scale. Of course it's expected to tend to infinity when l_{CG} tends to zero (to coincide with the analytical solution provided by [Williams, 1957] without coarse-graining). In fact, a tendency stating $\sigma_f \sim \frac{1}{\sqrt{l_{CG}}}$ is found. Similar expressions relating the tensile strength σ_f to the characteristic length l_c , E and g_c are found in [Nguyen et al., 2016, Benallal and Marigo, 2007, Pham et al., 2011b, Amor et al., 2009] for gradient and non-local damage models, and in the findings from the previous Chapter 1 (unidimensional solution of the phase-field model). Interested readers are also referred to Section 3.7 in Chapter 3 for similar findings also on heterogeneous phase-field simulation results.

On the presence of a damage law

As the quasi-brittle behaviour under mode I loading of the effective material is set - independently of l_{CG} - an attempt to write a damage evolution law based on the effective stress-strain (Figure 2.9) results and the standard degradation function $g(\alpha) = (1 - \alpha)^2$ (found in Chapter 1) was made. Interested readers are referred to Appendix C. However, difficulties were encountered when extending the scheme to a combined mode I mode II loading, even for mode I with $T - stress$ loading. Future prospects require building on these findings to further advance on linking damage mechanics to fracture mechanics.

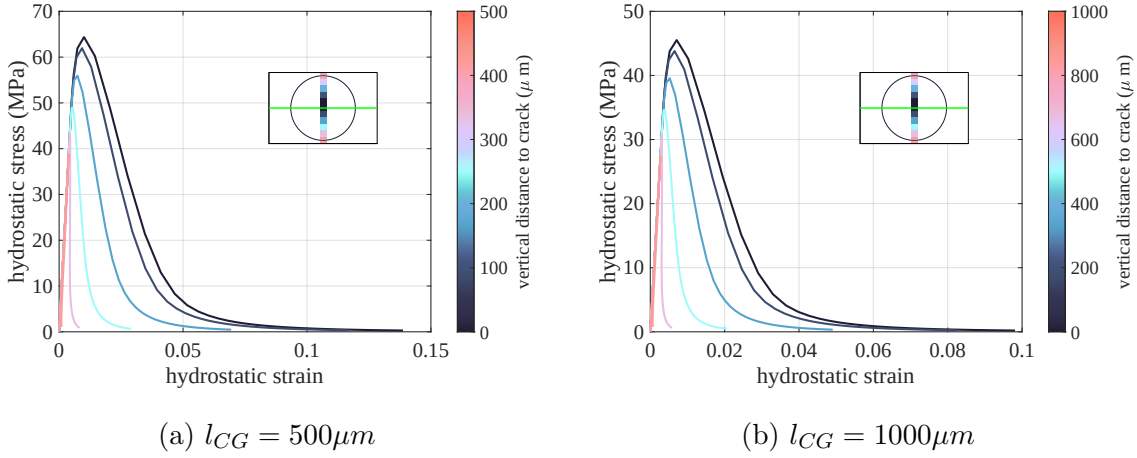


Figure 2.9 – Coarse-grained stress-strain behaviour of the data points as a function of their vertical distance to the crack path at two length scales l_{CG} . In the schematic, the crack path is represented by the green horizontal line, and the circle represents the coarse-graining function width

2.7 Concluding remarks

In this chapter, we introduced the coarse-graining technique as an upscaling method that does not require specific boundary conditions (as opposed to classical homogenisation schemes) and that should be indeed applicable to non-periodic structures presenting high strain localisation.

It's a *bottom-up* approach adapted from Molecular Dynamics studies, and it allows the evaluation of continuum quantities at different scales starting from the scales of heterogeneities.

The coarse-graining method is solely based on a definition of a coarse-grained mass density and a manipulation of the inviolable conservation laws:

- (i) The balance of mass
- (ii) The balance of linear momentum

It allows the consistent computation of continuous fields across the scales without any *a priori* on the behaviour at the larger scales:

- (i) Densities,
- (ii) Velocities,
- (iii) Displacements,

- (iv) Strains and strain rates, and
- (v) Stresses

We validated our implementation to determine the effective elastic properties of a Periodic lattice of holes and compared the results with other standard *RVE*-based homogenisation method. The second application validates the applicability of this method in cases where sharp localisation exists, by coarse-graining mechanical displacement and stresses obtained from near-tip asymptotic solution ([Westergaard, 1939]).

Successful bridging between fracture mechanics and damage mechanics is achieved: ***Quasi-brittle behaviour*** The coarse-graining method introduces a length scale which implies softening of the material - and thus an equivalency to a softening behaviour with a process zone, without any *a priori* on the behaviour at the larger scales. Plotting the stresses against the strains shows a typical response of quasi-brittle materials where a linear elastic region is followed by a non-linear region before softening. The notion of strength is thus notable.

Non-local effects Without any assumption on the material behaviour, the absence of a unique behaviour law that links the local variables, i.e., local strains and local stresses, is illustrated. The stress-strain history of the elements at different distances to the crack path is different suggesting thus non-locality of the behaviour.

After advancing the computational methods, introducing our contribution and validating their implementation on benchmark cases / simple examples, the following part tackles the multi-scale analysis of failure in architected materials. The analysis would evolve from phase-field modelling at the microscopic scale (scale of heterogeneities in the architected materials) to simulate brittle failure, towards the estimation of the effective elastic, toughness and strength properties of the material at the mesoscopic scale, via the herein proposed coarse-graining technique.

PART III

**Multi-scale analysis of fracture and
dynamic fracture**

MULTI-SCALE CRACK PROPAGATION IN ARCHITECTURED MATERIALS

Contents

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3.1 Introduction

The ability of architected materials to give a wide range of stiffness, strength and fracture toughness popularised their use. Demands on custom-designed architectures to meet certain specifications have boomed, and with them research activities around this subject. In this chapter, we address the crack propagation behaviour of three architected materials: a hexagonal lattice of holes and two Penrose-type-Quasi-Periodic distributions.

The remarkable properties of general architected materials regarding crack initiation and propagation were put forth by [Glacet et al., 2018]. In fact, previous work shows how toughness heterogeneities [Dalmas et al., 2009, Chopin et al., 2011, Patinet et al., 2013, Lebihain, 2019], elastic inclusions [Xia et al., 2013, Wang and Xia, 2017] or residual stresses [Bower and Ortiz, 1993, Lacondemine, 2019] induce trapping mechanisms, i.e., the crack is attracted to the architectures' patterns and trapped inside the tessellation. A new initiation is then required for the cracking to advance. This trapping mechanism is responsible for the better performances of the architected materials regarding fracture.

However, the real-life use of such highly heterogeneous materials is bridged by some limitations, in fact, despite the many powerful computational methods that have been developed in the last few decades, explicitly modelling the architectures for numerical simulations remains a heavy task. Thus, of course, it's appealing to describe a simpler nature of those materials.

In this spirit, this chapter tackles the crack propagation inside architected materials.

A multi-scale analysis of the propagation via the coarse-graining approach proposed in Chapter 2 is applied on crack propagation simulations. The coarse-grained mechanical response is investigated at multiple intermediate scales l_{CG} , i.e., between the scale of heterogeneities and the supposedly effective material.

This application elaborates on the indispensable ingredients for accurately accounting for the microstructural influence at larger scales (e.g., scales of the part). By analysing the coarse-grained mechanical response before fracture and through the crack propagation, the effective crack path, fracture strength and fracture toughness of the architected material regarding the propagating crack are established. The 'homogeneity' of these properties are analysed across the scales, and discussions regarding the inevitability of considering an effective non-homogeneous material in which the influence of substructures is preserved at the mesoscopic scales are advanced.

This chapter is organised as follows: first, the numerical model for the micromechanical

simulations is advanced. Results from the phase-field simulations are presented in Section 3.2. After acquiring the microscopic fields (fields from simulation in which the microstructures are explicitly modelled), the coarse-graining technique is initiated. The analysis of the effective density and effective elasticity fields are presented in Sections 3.3 and 3.4. A multi-scale analysis of the effective crack path shows a conservation of the crack tortuosity in the Quasi-Periodic material even for large observation scales (Section 3.5). The notion of strength emerging from the obtained coarse-grained stress-strain response is analysed across the scales in Section 3.6. Last, the evolution of the effective toughness is analysed in Section 3.7.

Remark 3.1. *Parts of this chapter are published in [Eid et al., 2021].*

3.2 Quasi-static fracture simulation

For the micro-mechanical simulations, the microstructures (Section 0.4, Figure 8, Table 1) are put at the core of a Tapered Double Cantilevered Beam (TDCB) fracture geometry to provide crack growth stability from the tapered profile of the specimen [Brown, 2011, Grabois et al., 2018]; the microstructure is surrounded by a homogeneous bulk material, the dimensions are put forth in Figure 3.1. Displacement boundary conditions are applied for the phase-field micro-mechanical simulation. In fact, the stability in crack growth provided by the TDCB specimen is believed to match the stability provided by the application of a surfing boundary condition [Hossain et al., 2014]. In both cases, the crack evolves as it pleases inside the microstructure. In this study, the former - more straightforward - approach is adopted.

We recall that in this chapter, we confine ourselves to the quasi-static evolution of cracks neglecting thus dynamics effects. The numerical discretization $h = 200\mu m$ is thoughtfully adapted to the heterogeneities sizes and distributions inside the domain and based on [Nguyen et al., 2016]; the internal parameter of the phase-field model l_c is set to $400\mu m$. Both lengths are much smaller than the structures' heterogeneities leading to mesh-independent crack initiation and propagation. Table 3.1 resumes the overall model and material parameters considered for the simulation.

Figures 3.2 displays the phase-field simulation results. A comparison with some experimental results¹ is also reported. The influence of the microstructures on the crack

1. Within a first year engineering project, three students worked on an experimental study of crack propagation in matching samples. Samples were cut-out via a laser-cutting machine from a commercial

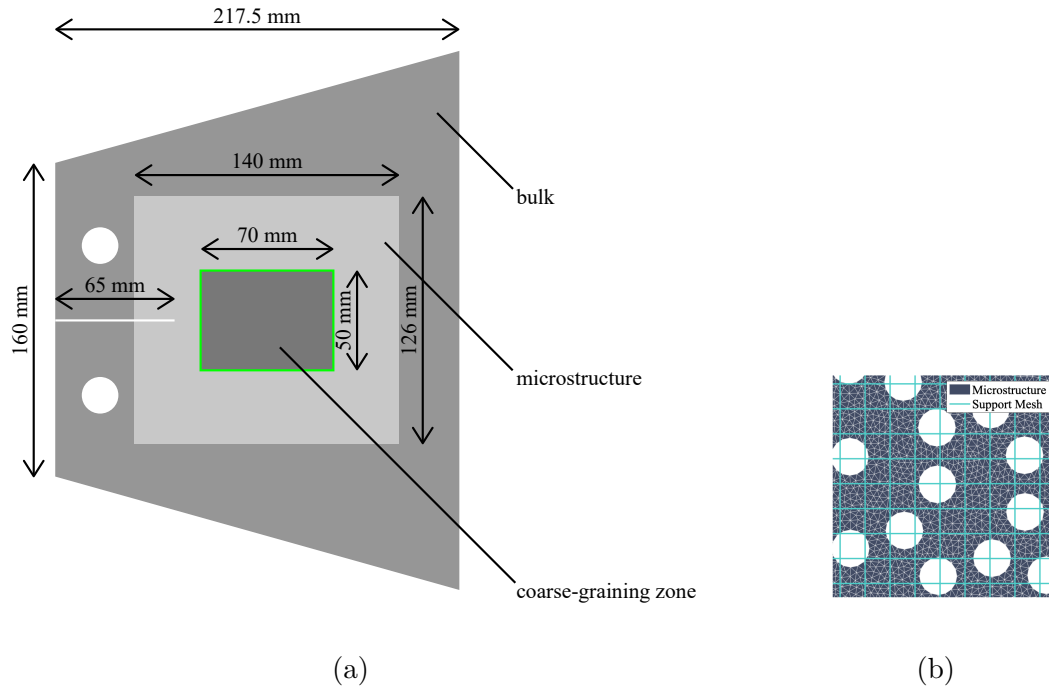


Figure 3.1 – Full (a) and close-up (b) diagrams of a typical finite element mesh of a TDCB specimen with the considered coarse-graining support mesh region (in light blue) allowing the study of large scales l_{CG} up to 10 times the mean distance between holes d .

Crack density function	Equation 1.3 ([Miehe et al., 2010a])
Strain split	Extensive/compressive ([Miehe et al., 2010a])
Plane strain assumption	
Boundary condition	Imposed $\underline{u}$
E (Young's Modulus)	$3GPa$
ν	0.35
g_c	$250J/m^2$
l_c	$2 \times \text{mesh size} = 2 \times h = 400\mu m$ ([Nguyen et al., 2016])
c (threshold)	0.25

Table 3.1 – Overall phase-field model and material parameters considered for the quasi-static simulations

propagation is prominent. For the Periodic material, a simple linear crack path is obtained (both numerically and experimentally) suggesting thus the presence of weak planes [Glacet, 2018, Réthoré et al., 2017]. For the Quasi-Periodic materials, each type proposes different-more tortuous paths suggesting more complexity of the damaging process. Even though experimental and numerical patterns don't exactly fit, (for reasons reported in the footnote ¹) the influence of the microstructure is reflected on both paths and is fundamentally similar: cracks tend to deviate around 'resilient patterns', an effect systematically reproduced at different locations inside the specimen both numerically and experimentally. A more detailed investigation on the crack paths is found in Section 3.5.

From the phase-field simulations, the macroscopic response -knowingly the load-displacement curve- was acquired. This give insight on the effective 'macroscopic' behaviour of the different microstructures' response. Unsurprisingly, the influence of the microstructure is reflected on the load-displacement response (Figure 3.3). Periodic oscillations are found in the Periodic microstructure and arbitrary oscillations are found in the Quasi-Periodic microstructures. The maximum load and the imposed displacement at which the maximum load is reached are virtually similar.

The energy dissipated in the respective materials, when the crack propagates inside a domain of interest Ω^0 inside the TDCB are given in the Table 3.2. Ω^0 is defined in Chapter 2 as the zone of interest for the coarse-graining computations. Considering only

PolyMethyl Methacrylate (PMMA) plate manufactured by Arkema. A reproduction of the exact specimens was of extreme difficulty due to the imprecision of the laser-cutting machine. Cut holes were more or less skewed. The laser beam cutting the PMMA generated residual stresses in the material. These uncontrolled phenomena lead to discrepancies in the fracture process making it hard to be numerically reproduced. Despite these difficulties, the simulation managed to qualitatively reproduce the crack patterns.

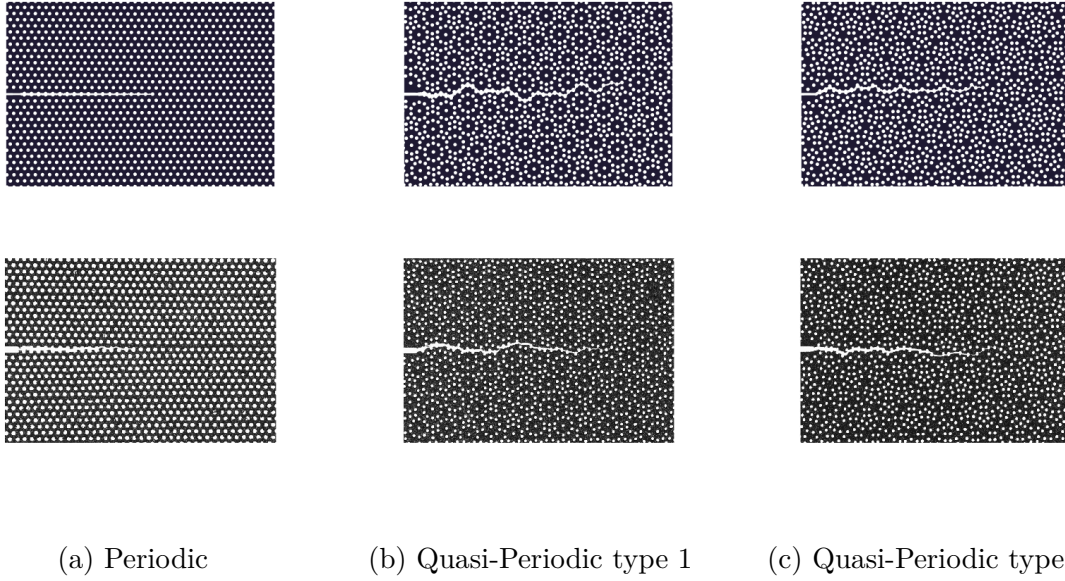


Figure 3.2 – Phase-field simulation of the fracture of the architected materials (up), the data points where the damage $\alpha > 0.99$ are removed to mimic a crack opening. Experimental footage showing the crack patterns obtained in-lab

the dissipation in this zone (coarse-graining support domain) allows a later-on comparison with the energy dissipation at the coarse-grained scales (in Section 3.7). The energy dissipated during the crack growth is defined as the difference between the variation of the work done by the external loads and the work of the internal forces during the growth of the crack area. The architected materials actually dissipate less energy than the full material; however, when related to the effective density and rigidity modulus, the hexagonal Periodic shows an improved toughness of 14% over the homogeneous materials while the Quasi-Periodic 1&2 show an overwhelming 30% improvement in their capacity

Geometry	Dissipated energy (mJ)
Homogeneous	347
Periodic	229
Quasi-Periodic - type 1	230.6
Quasi-Periodic - type 2	228.5

Table 3.2 – Energy dissipated by the crack propagation in the coarse-graining support domain computed from the load-displacement curve

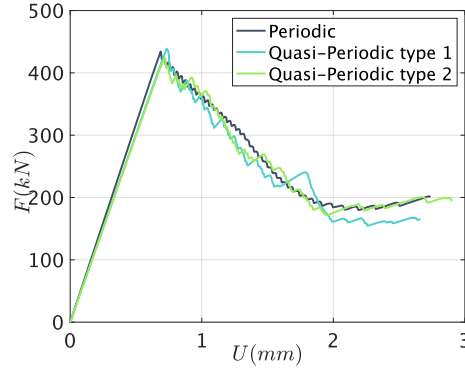


Figure 3.3 – Load-displacement response from the phase-field simulations of the TDCB samples embedding the three architectures

to dissipate energy for a crack of same overall length as in the bulk material.

After acquiring the simulation results, the coarse-graining is resumed. The domain of interest Ω^0 is considered for the study and then subdivided into finite constant-stress-constant-strain elements of size $H = 1mm$ without loss of generality (Figure 3.1(b)). The considered coarse-graining function then sweeps over the mesh support constructing a database of mechanically and physically consistent fields at multiple larger scales to be analysed without any a priori on the model at each scale and by considering the physics happening at the scale of heterogeneities. Ω^0 is at the core of the microstructure which allows the use of large l_{CG} and therefore large observation scales.

Exploiting the adapted coarse-graining method, one is able to investigate the microstructure at different transitional scales by building physically consistent density, displacement, strain and stress fields at each scale.

3.3 Density

As established in the method, the density field $R(x)$ is first computed. Effective density fields of the Quasi-Periodic type 1 microstructure at different coarse-graining scales l_{CG} are presented in Figure 3.4. Results actually show the ability of the method to construct heterogeneous/homogeneous continuous density fields depending on the scale of interest without any a priori on the effective field's homogeneity. To analyse the 'homogenisation' of the effective density as the coarse-graining scale l_{CG} is increased, we plot the evolution of the mean and the coefficient of variation of R for the three considered microstructures (Figure

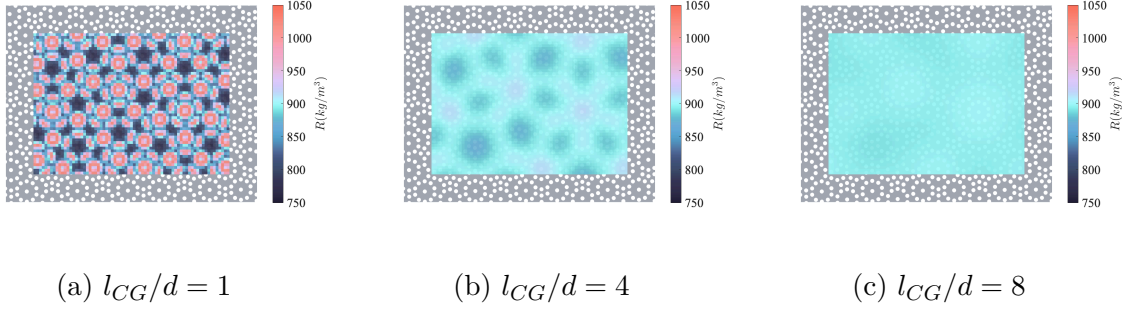


Figure 3.4 – Effective density fields of type 1 Quasi-Periodic microstructure for three different scales.

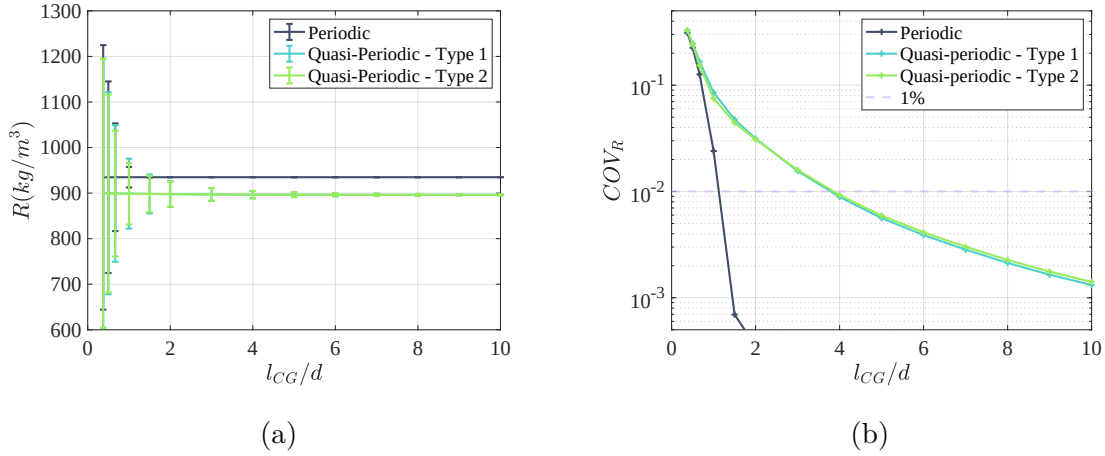


Figure 3.5 – Density conservation through mesoscales (a) and the evolution of the corresponding coefficient of variation COV_R - defining the heterogeneity of the effective density - evolution with l_{CG} (b)

3.5 (a)). It's considered that the homogeneity of a field is attained once its corresponding coefficient of variation COV drops below the $\leq 1\%$ threshold. The arithmetic mean is calculated as the sum of the sampled values (whether at the nodes or the Gaussian points of the coarse elements in Ω^0) divided by the total number of samples (nodes and Gaussian points respectively). The standard deviation is found by taking the square root of the average of the squared differences of the values from their mean value. The coefficient of variation is defined as the ratio of the standard deviation to the arithmetic mean (Chapter 2).

As the implemented coarse-graining method is based on the inviolable conservation laws - mass continuity between them -, it can be seen that the mean effective density in the studied domain is conserved through the scales and only the homogeneity of the field is altered. The heterogeneities of the effective density of the material are smeared-out much faster when considering a Periodic microstructure at $l_{CG}/d = 1$, while the Quasi-Periodic microstructures require higher coarse-graining scales for the density heterogeneities to smear-out at $l_{CG}/d = 4$ (Figure 3.5 (b)).

3.4 Elastic Properties

Once the density fields are computed, manipulating the balance of mass at the fine and the coarser scale leads to the computation of the effective displacement fields that can be differentiated to determine the strain fields. The balance of linear momentum allows the evaluation of the effective stress fields. First, we aim to determine the behaviour of the material prior to damaging. For this purpose, we put the microstructure at the core of a rectangular specimen on which two tensile and one shear test simulations are conducted. From the microscopic mechanical fields, coarse-grained displacements, strains and stresses can be evaluated for different l_{CG} . Coarse-grained strain and stress couples in Ω_0 (obtained from the three tests) provide an evaluation of the nine components C_{ij} of the effective stiffness tensor $\mathbb{C}$, representative of the elastic behaviour, at each material point for the considered scales. It was observed that in the specimen coordinate system, the shear-extension coupling terms vanish; the reduced expression for the effective elasticity

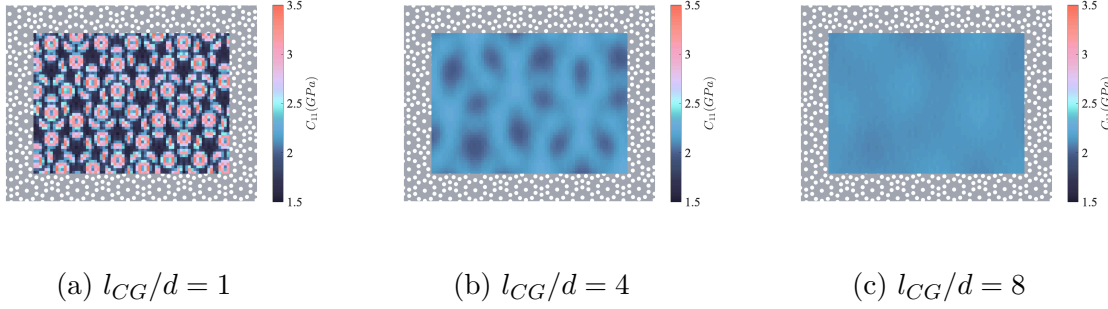


Figure 3.6 – Fields of the C_{11} component of the effective elasticity tensor of type 1 Quasi-Periodic microstructure at three different scales.

tensor written in (3.1) is thus adopted:

$$\begin{bmatrix} S_{11} \\ S_{22} \\ S_{12} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{21} & C_{22} & 0 \\ 0 & 0 & C_{66} \end{bmatrix} \begin{bmatrix} E_{11} \\ E_{22} \\ 2E_{12} \end{bmatrix} \quad (3.1)$$

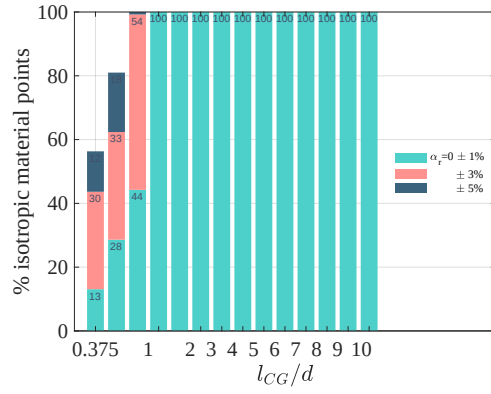
Fields of the C_{11} component of the effective elasticity tensor of the Quasi-Periodic type 1 microstructure at three different coarse-graining scales l_{CG} are presented in Figure 3.6; the heterogeneity of C_{11} is shown to persist for large regularisation scales and thus the influence of the distribution of holes on the effective stiffness fields. From the computed effective elasticity tensors, both the anisotropy and homogeneity can be evaluated. As mentioned previously, the symmetry order of the studied Periodic and Quasi-Periodic microstructures (6 and 5-fold symmetry respectively) are expected to lead to an equivalent isotropic response. From here, we aim to determine the scale from which the symmetry orders actually governs the elastic isotropy. To do so, the two-dimensional elastic anisotropy index a_r - defined in [Li et al., 2020] - is analysed at each material point for each observation scale. An explicit expression of a_r as a function of C_{ij} and S_{Cij} can be written as follows:

$$a_r = \left(\left[\frac{1}{4}(C_{11} + C_{22} + 2C_{12})(S_{C11} + S_{C22} + 2S_{C12}) - 1 \right]^2 + 2 \left[\frac{1}{16}(C_{11} + C_{22} - 2C_{12} + 4C_{66})(S_{C11} + S_{C22} - 2S_{C12} + S_{C66}) - 1 \right]^2 \right)^{\frac{1}{2}} \quad (3.2)$$

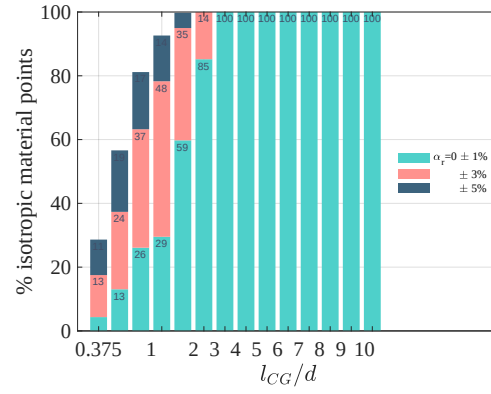
Where S_{Cij} represent the components of the compliance tensor $\mathbb{S}_{\mathbb{C}}$ defined as $\mathbb{S}_{\mathbb{C}} = \mathbb{C}^{-1}$.

a_r takes the value of 0 in the case of perfect isotropy. Otherwise, a_r increases as the anisotropy strengthens. The main advantage of a_r over other anisotropy indices (Kube [Kube, 2016], Zener [Zener, 1947],...) is its direct applicability in 2D, for any symmetry type, and its direct evaluation from the elasticity tensor. In this study, a_r is computed from the evaluated elasticity tensors $\mathbb{C}$ and $\mathbb{S}_{\mathbb{C}}$ at each material point of the domain for each coarse-graining scale l_{CG} . The distribution of these indices is shown in Figure 3.7. It's observed that for the Periodic material, all the points present an isotropic response (with an error lower than 1%) once l_{CG} is larger than the characteristic length d of the microstructure. Although the material symmetry order of the Quasi-Periodic materials considered suggests elastic isotropic behaviour, it's quite clear that this isotropy of the elasticity tensor cannot be reached at small scales but in fact, suggests a required scale of observation of at least 3 times the characteristic length d of the microstructure where the anisotropy indices of all the material points fall within 1% to 0 corresponding to the isotropy of the elasticity tensor in the whole domain.

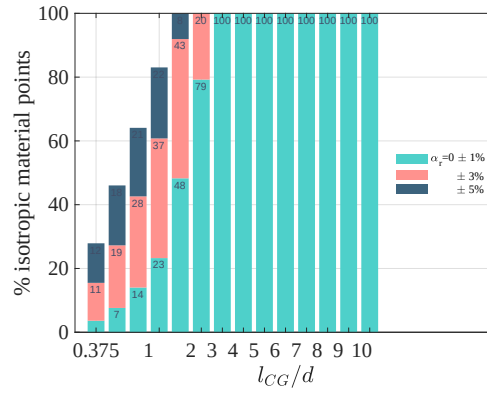
Next, the homogeneity of the elastic moduli is put forth at different l_{CG} . Only the observation scales at which the effective elasticity in the whole domain is isotropic (within 1% error) are considered in the study (Figure 3.7), i.e., $l_{CG}/d \geq 1$ for the Periodic microstructure and $l_{CG}/d \geq 3$ for the two Quasi-Periodic microstructures. From the isotropic elasticity tensors fields, effective Young modulus (E) and Poisson ratio (ν) are computed for different l_{CG} on each element in the domain Ω_0 . Statistical analysis is conducted on the evaluated effective elastic moduli to identify their possible 'homogenisation' for each microstructure. The mean and standard deviation of the two material properties are plotted in Figures 3.8 and 3.9 as well as the evolution of the coefficient of variation of each property with the coarse-graining scale. The Poisson ratio converges and homogenises at considerably low length scales of observation. For the Periodic microstructure, the effective Young modulus is homogenised at considerably small observation scales ($l_{CG}/d = 1.5$). The average effective Young modulus for the different microstructures rapidly converges, contrary to its variation, especially for the Quasi-Periodic microstructures where the effective Young modulus field requires larger length scales, at least 7 times the characteristic length d , to homogenise. Next, we proceed with the multi-scale damage analysis, starting with the influence of the observation scale on the crack path towards the effect on the strength and toughness fields as the crack advances inside the microstructures.



(a) Periodic



(b) Quasi-periodic type 1



(c) Quasi-periodic type 2

Figure 3.7 – Material points distribution based on the elastic anisotropy index a_r computed at different coarse-graining scales for the considered microstructures.

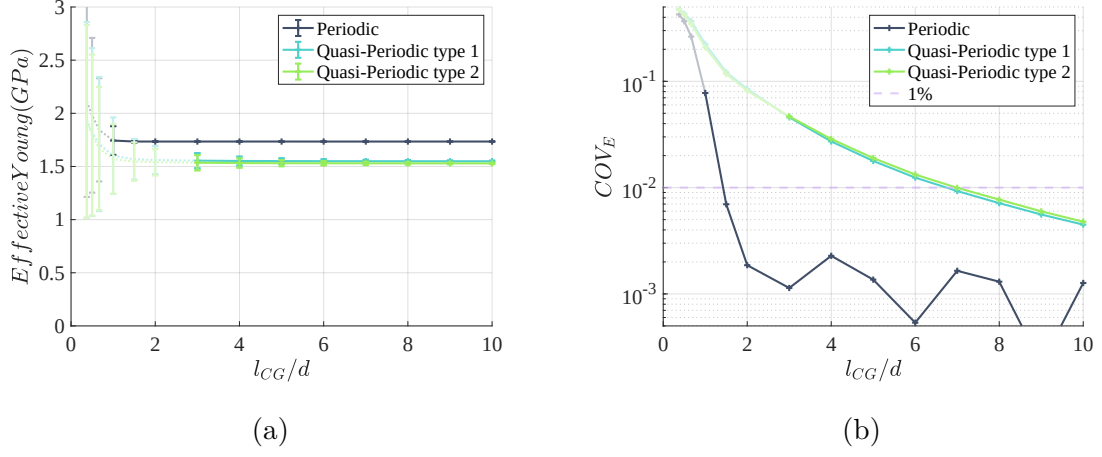


Figure 3.8 – The effective Young modulus computed at different l_{CG} for the three microstructures (a) and the evolution of the corresponding coefficient of variation COV_E - defining the heterogeneity of the effective Young modulus - with l_{CG} (b)

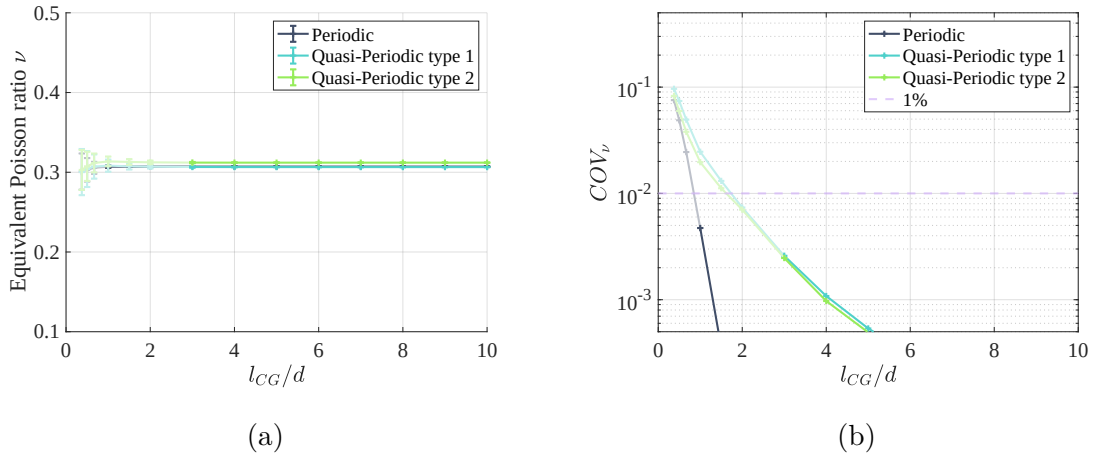


Figure 3.9 – The effective Poisson ratio computed at different l_{CG} for the three microstructures (a) and the evolution of the corresponding coefficient of variation COV_ν - defining the heterogeneity of the Poisson ratio - with l_{CG} (b)

3.5 Crack Path

Displacement and stress fields from the phase-field simulations of fracture on the TDCB are upscaled, and coarse-grained displacements, strains and stresses with damage consideration are obtained. As the crack advances in the microstructure, interactions between the crack and the structure of the material are observed, especially in the Quasi-Periodic microstructures. The crack can be expected to follow the path that would allow the maximum dissipation of energy. For type 1 Quasi-Periodic distribution, 'resilient patterns' (bittersweet circles in Figure 3.10(b)) impose the deviation of the crack. For the type-2 Quasi-Periodic distribution, kinking of the crack is present, and due to the high amount of elastic energy stored in the specimen before kinking (bittersweet circles in Figure 3.10(c)), failure becomes unstable. The question arising here regards the ability to replace the complex crack path (at the microscopic scale) by an equivalent failure band (at larger scales of observations) represented by an effective straight crack path. To answer that question, the effective crack path at the coarse-grained scale is determined. Without loss of generality, we define the effective crack tip at time $t = t_0$ as the local zone where the maximum stress occurs at this time $t = t_0$. By considering different criteria (Rankine, Maximum Volumetric Stress, ...) to evaluate the position of maximum stress, identical results were obtained; that is of course due to the stress singularity at the crack tip. The choice of the Rankine criterion naturally emerges for the description of brittle and quasi-brittle failure. From here, the effective 'mesoscopic' crack tip position is defined as the local zone where the maximum mesoscopic Rankine stress is reached for each microscopic crack tip position. The length scale introduced via the coarse-graining l_{CG} method suggests softening of the material (Figure 3.13 - more details about the stress-strain response is found in Section 3.6)- and an equivalency to a process zone is present suggesting that the critical stress before softening happens at a distance to the true crack tip (the crack tip determined from the micromechanical simulations). The evolution of the crack paths and their corresponding tortuosity at different scales in the Quasi-Periodic microstructures are shown in Figure 3.10. Counter intuitively, one can observe prominent tortuosity of the crack path even at large scales. In fact, for the type 1 Quasi-Periodic microstructure, the crack tortuosity only drops of less than 6% at $l_{CG}/d = 10$ while the type 2 crack path tortuosity drops around 9% from its microscopic value (Figure 3.10(a)). The conservation of the tortuosity across the considered scales drops the idea of the consideration of an effective straight failure band to replace complex crack paths. *FFT* analysis on the crack paths

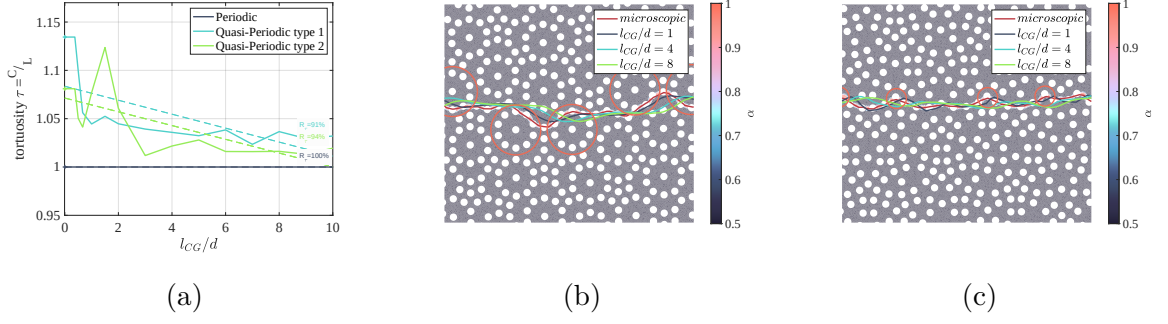


Figure 3.10 – Mesoscopic crack paths for the type 1 (b) and type 2 (c) microstructures at different l_{CG} and the corresponding crack tortuosity evolution with l_{CG} (a).

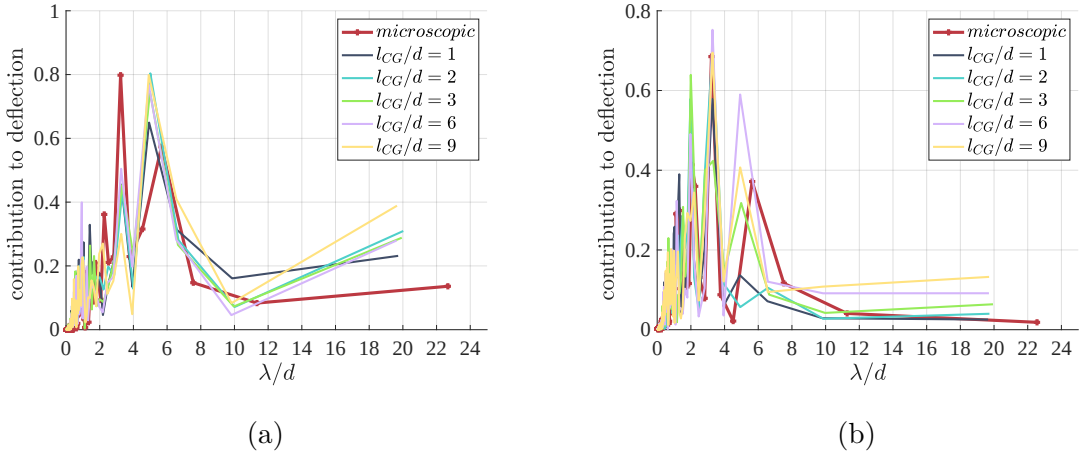


Figure 3.11 – FFT analysis on the mesoscopic crack path inside the Quasi-Periodic type 1 (a), and Quasi-Periodic type 2 (b) microstructures

at different observation scales offers an insight on the amplitudes and wavelengths that contribute to the effective crack deflection. Later, the interaction between the wavelengths driving the crack deflection and the wavelengths driving the variations of the critical stresses and energy dissipation along the crack path are confronted. Figure 3.11 shows the *FFT* analysis results on the crack path inside the two Quasi-Periodic microstructures. As expected, small wavelengths $\lambda/d \leq 3$ are smeared-out as the coarse-graining scale increases and more weight on the larger wavelengths is observed $\lambda/d \geq 10$. The type 1 response shows decaying amplitudes at wavelengths $\lambda/d = 2 - 3$ with a drop of about 62% (Figure 3.11(a)). The contribution of the wavelengths around $\lambda/d = 5$ corresponding to the distance between zones of 'resilient patterns' (Figure 3.10(b)) is conserved through the scales and is responsible for 80% of the crack deflection. For the type 2 Quasi-Periodic microstructure, one clearly observe the absence of uniquely conserved high amplitude wavelengths across the scales (Figure 3.11(b)), except for $\lambda/d = 2 - 3$ that actually corresponds to the kinking spots. The crack path, in comparison with the type 1 -except for the kinking spots- does not conserve the same wavelengths suggesting a more easily smoothed crack path. Next, we focus on the influence of the microscopic heterogeneity on the resistance and toughness fields at different coarse-graining scales, and we confront the wavelengths controlling the heterogeneities with the wavelengths present in the crack paths.

3.6 Fracture strength

Displacement and stress fields from the phase-field simulations of fracture on the TDCB specimens with the microstructures at their cores are upscaled, and coarse-grained displacements, strains and stresses with damage consideration are obtained. Figure 3.12 shows the vertical displacement field at different coarse-graining scales. The jump on the crack faces are smoothed as the observation scale increases and the sharpness of the crack at these scales is expected to be smeared out. A plot of the stress-strain relation computed at the coarse-grained scales of a TDCB test corresponds to a stress-strain response of a quasi-brittle behaviour (Figure 3.13, analysis similar to Chapter 2, Section 2.6.2). Here, the history of the hydrostatic stresses as a function of hydrostatic strains is plotted for different points in Ω_0 .

As shown in Figure 3.13, the material undergoes a linear elastic trend followed by a non-linear region before reaching the critical stress where softening occurs. For small length scales, the increased width of the peak in the linear elastic region suggests heterogeneity

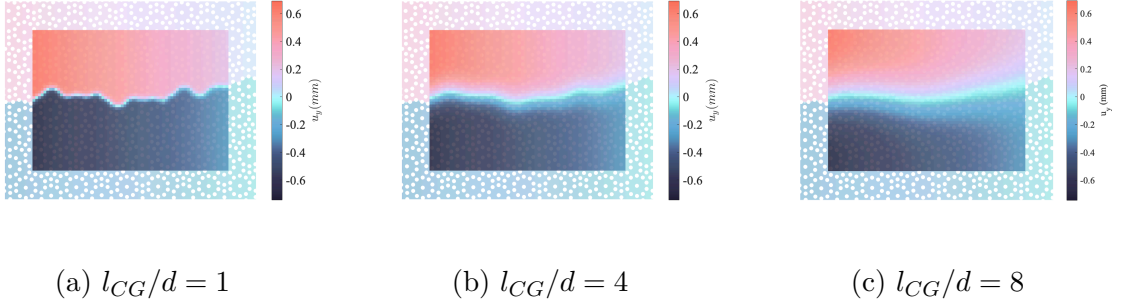


Figure 3.12 – Upscaled vertical displacement U_y at different l_{CG} . The discontinuity of the displacement field is regularized by the coarse-graining function and dictated by its width

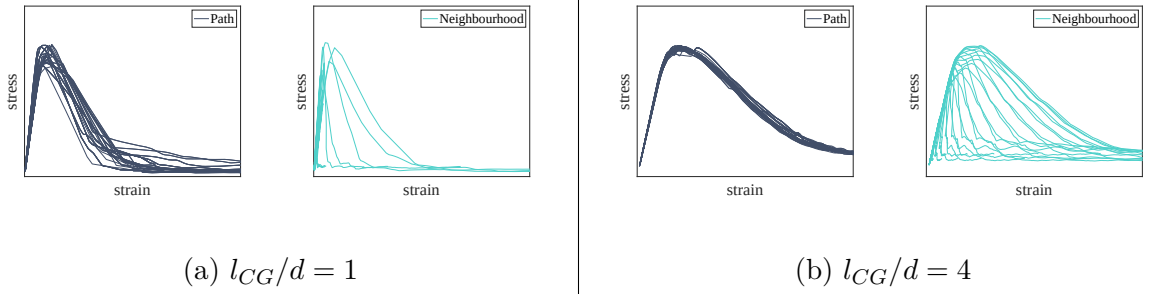


Figure 3.13 – Stress-strain behaviour of elements along the crack path and in a neighbourhood of the crack at two length scales l_{CG}

of the modulus, to confirm the previous results regarding the homogenization of the elastic properties of the materials. The curve reaching the maximum stress corresponds to the response of the elements along the crack path. As the distance to the crack path d_c increases, the stress-strain response of the corresponding elements reach lower maximum stress states followed by some softening. When the elements are much further to the crack path, they remain undamaged and show typical linear elastic stress-strain response (Section 2.6.2). For instance Figure 3.13 shows the stress-strain response of a material in the neighbourhood of a crack at a specific abscissa in the domain, at $l_{CG}/d = 1$ which corresponds to $l_{CG} = d = 3mm$. As the coarse-graining mesh size H is equal to $1mm$, we find 6 different stress-strain responses of the elements corresponding to the discretization of the damageable zone. The same trend is found at different coarse-graining scales l_{CG} (Figure 3.13(a)) where a unique relation between the local stress and local strain states does not exist. Instead, as we move further from the crack path, and due to the regularizing nature of the coarse-graining, softening persists yet starts at lower critical stress levels

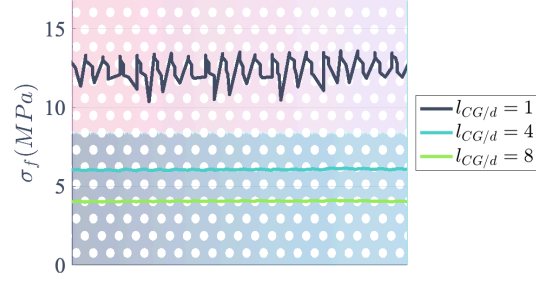
leading thus to non-unique relations between the stresses and strains.

Remark 3.2. *If in Chapter 2, Figure 2.9 we didn't have different numbers of (stress-strain) curves for different coarse-graining scales l_{CG} , it is because in that case we adapted the coarse-graining mesh size H as a function of l_{CG} , fixed at $H = l_{CG}/5$. This of course would alter the resolution of the mesoscopic fields. Here, we fix the coarse-graining mesh size H and analyse the influence of l_{CG} without altering the resolution of the fields.*

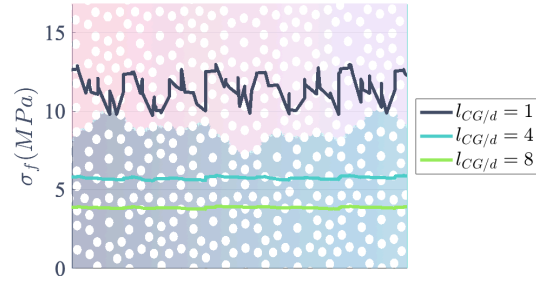
Moreover, when following the stress-strain response of the elements along the crack path, especially at low scales, and as the crack propagates through different patterns in the microstructure, the critical stress state reached before softening is found to differ from one position to another along the path. We define the maximum Rankine stress reached at each position of the crack tip as the *fracture strength* or simply *strength* denoted σ_f , without abuse of language. The evolution of the critical Rankine stress at different scales of observation is plotted in Figure 3.14 for the Periodic (a), Quasi-Periodic type 1 (b) and Quasi-Periodic type 2 (c). The below figures thus show the significant influence of the local differences inside the microstructure - distribution of holes - on the fracture strength of the effective continuum. As the crack gets trapped inside the holes, much higher loading is required for the crack re-initiation, this phenomenon is mainly observed on the Periodic geometry at the smallest scales, while for the Quasi-Periodic geometries, not only crack trapping influence the critical stress state reached, but also the crack deflection and deviation around the special 'resilient patterns'.

The strength fields at different coarse-graining scales l_{CG} are studied and both the average critical stress and its coefficient of variation over the crack path for each length scale l_{CG} are plotted in Figure 3.15. It's clear that the critical stress σ_f decreases when l_{CG} increases.

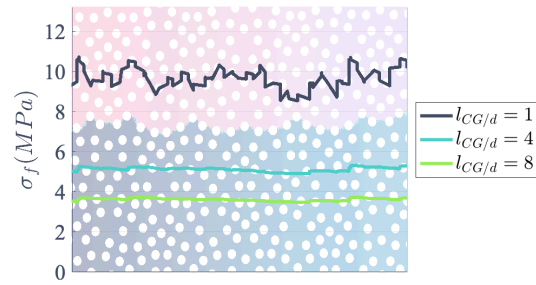
In Figure 3.15, one observes higher strength for the Periodic microstructure in comparison with the two Quasi-Periodic microstructures. A study on the evolution of the 'homogeneity' of the strength is also conducted. Here, the coefficient of variation is evaluated by considering the squared differences of the values from the normalised values of a homogeneous response - allowing the study of the deviation of the strength surpassing the geometrical influences of the TDCB geometry and the loading conditions. Unlike the elasticity, the effective strength of the microstructures remains highly heterogeneous even at large l_{CG} . From Figure 3.15(b), it's clear that the coefficient of variation stabilizes and slightly increases at large scales of observations independently of the microstructure. The coefficient of variation of the strength of type 1 and the type 2 microstructures stagnates



(a)



(b)



(c)

Figure 3.14 – Fracture strength σ_f evolution along the crack path for the Periodic (a), Quasi-Periodic type 1 (b) and Quasi-Periodic type 2 (c) microstructures.

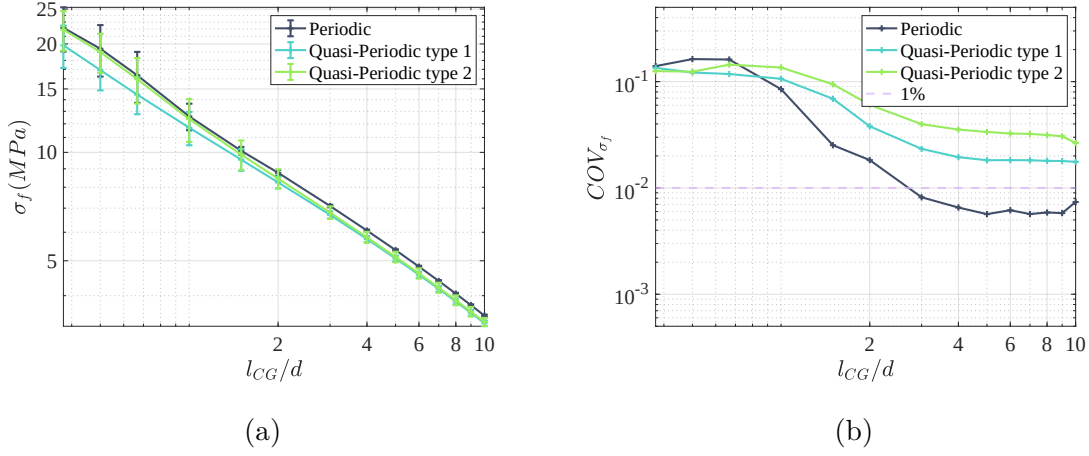


Figure 3.15 – Evolution of the mean fracture strength σ_f as a function of l_{CG} for the three microstructures (a) and the evolution of the corresponding coefficient of variation COV_{σ_f} defining the heterogeneity of the effective strength field of the continuum (b)

at about 2% and 3% respectively. The Periodic's COV_{σ_f} converges to 0.6%. Counter-intuitively, the coefficient of variation of the effective strength of the type 1 microstructure is lower than that of type 2 even though the path is more complex, but this may be caused by the presence of kinking in specific places leading to a huge increase of the loadings before the crack saps in comparison to the rest of domain where the crack path is smooth and straight.

Looking at Figure 3.14, it's hard to quantify both the microstructural effects and the influence of l_{CG} on the fracture strength evolution in the material. For this purpose, the fracture evolution is studied in the frequency domain, and *FFT* analysis allows to display the wavelengths and amplitudes to better depict the interactions of the microstructures and the coarse-graining impacting the strength. Figure 3.16 compares the wavelength spectrum of the *FFT* analysis transformed from the fracture strength's deviation D_{σ_f} . The amplitude is computed as the ratio of the amplitude of each wavelength to the *RMS* (root mean square) amplitude of the input signal. The Periodic microstructure analysis shows a dominant peak occurring at a wavelength $\lambda = d$ corresponding to the length scale of the microstructure. The relatively low (30%) drop of the contribution from the small scale to the largest considered scale of $\lambda = d$ suggests that the variation of the strength σ_f of the material is controlled mainly by the distance d between the holes even on large observation scales for a Periodic microstructure. This observation could explain the stagnation of COV_{σ_f} across the scales. As seen previously on the crack path analysis,

more weight is put on the larger wavelengths as the coarse-graining scales increase. The size of the holes does not present any influence on the strength variations. Regarding the type 1 Quasi-Periodic microstructure in Figure 3.16(b), one clearly observes the drop of the contributions of the small lengths scales and the rise of the contributions of the larger wavelengths as the coarse-graining scales increase. The peaks on the wavelengths around $\lambda/d = 2 - 3$ persist with increased influence as the scale of observation enlarges. Comparing the *FFT* analysis of the crack path and the strength offers insights on the link between the wavelengths controlling the crack inside the microstructure and the effective strength. As the crack deflects mainly every $\lambda/d = 5$, it would have travelled two 'resilient patterns' zones. This reflects the periodicity of the crack path that is twice the periodicity of the mechanical response. Once again, we can see that the main variation of the strength of the material is directly controlled by the distribution of holes. For the type 2 Quasi-Periodic microstructure (Figure 3.16(c)), even at the smallest scales, the heterogeneity of the strength comes from the long-range variations. At the smallest scale, 50% of the deviation comes from the larger wavelengths, which is due to the kinking that happen for the crack inside this microstructure at wide distances in the domain. Moreover, the small peak present at the small scale at $\lambda/d = 1$ corresponds to the crack travelling from one hole to another in a straight path between the kinking zones. The other small peak at $\lambda/d = 2 - 3$ (also met in type 1 microstructure) decays as the scale is increased. As the coarse-graining scale enlarges, the small wavelengths contributions are smeared out leading to the extreme rise of the influence of the large scales onto the strength variations.

3.7 Fracture toughness

The difference in the loading history of the material points inside the microstructure - whether distributed along their crack path or in the neighbourhood of a crack (Figure 3.13) - is directly related to the total amount of energy absorbed by the material points until fracture. Here, the focus is on the energy absorbed by the material points along the crack path. The *effective toughness* G_d is defined as the energy to total failure evaluated as:

$$G_d = \int_0^{t_f} \underline{\underline{S}} : \underline{\underline{\dot{E}}} dt \quad (3.3)$$

allowing thus the measure of the energy dissipated per unit volume from the start of the loading ($t = 0$) until the fracture of the specimen ($t = t_f$). $\underline{\underline{S}}$ is the mesoscopic stress tensor and $\underline{\underline{\dot{E}}}$ is the mesoscopic strain rate tensor. The evolution of G_d at different scales

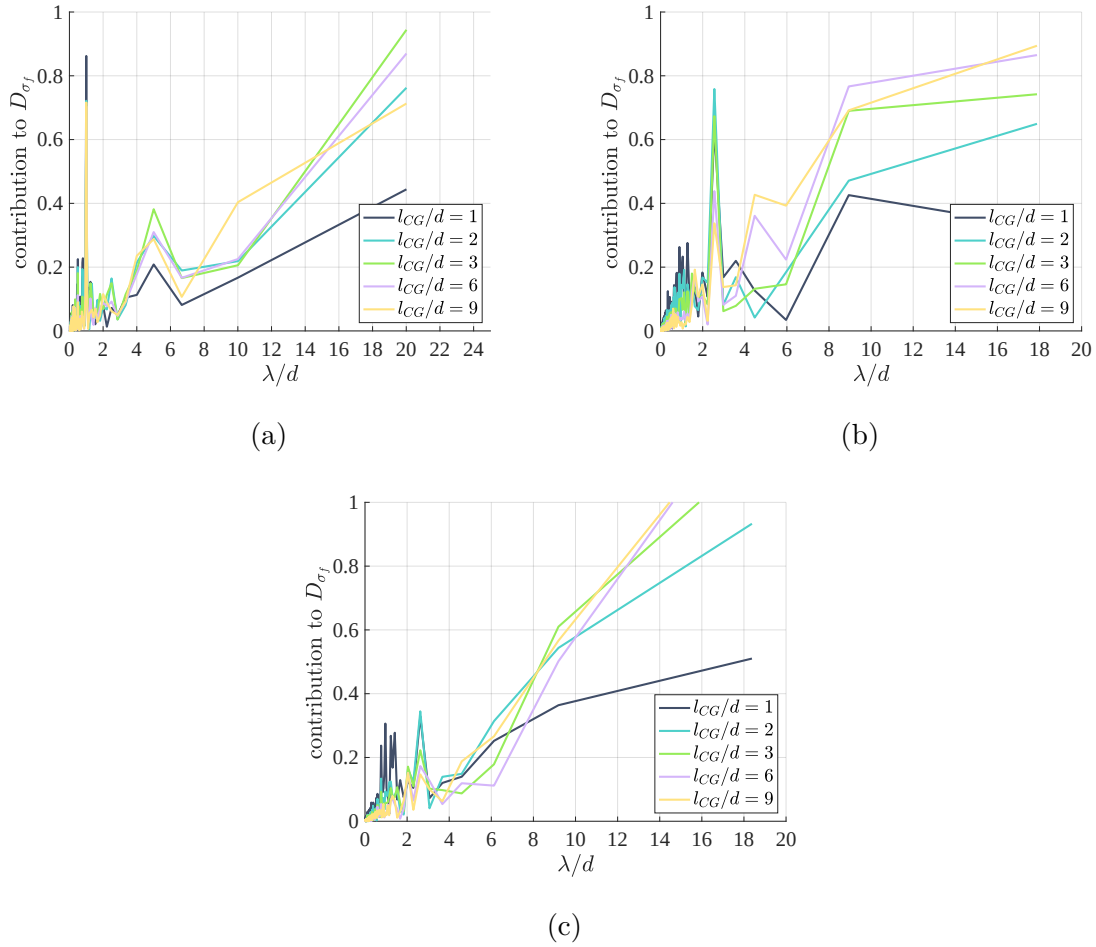


Figure 3.16 – FFT analysis on the fracture strength σ_f for the Periodic microstructure (a), Quasi-Periodic type 1 (b) and Quasi-Periodic type 2 (c) microstructures.

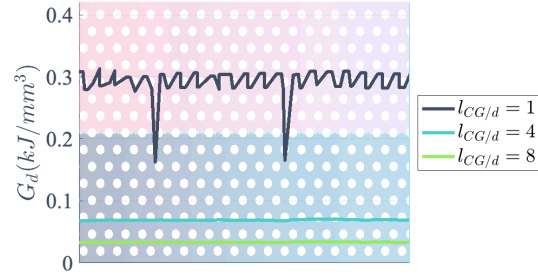
of observation is plotted in Figure 3.17 for the Periodic (a), Quasi-Periodic type 1 (b) and Quasi-Periodic type 2 (c). The below figures thus show the significant influence of the local differences inside the microstructure -holes distribution- on the overall dissipated energy along the crack path of the obtained continuum. As the crack gets trapped inside the holes, much higher energy is required for the crack re-initiation, this phenomenon is mainly observed on the Periodic geometry at the smallest scales, while for the Quasi-Periodic geometries, not only crack trapping influence the energy dissipation, but also the crack deflection and deviation around the special 'resilient patterns'.

A similar analysis to the one in Section 3.6 is conducted: a study of the evolution of this toughness parameter G_d at different coarse-graining scales followed by an *FFT* analysis to better understand the relationship between the microstructure and the effective toughness.

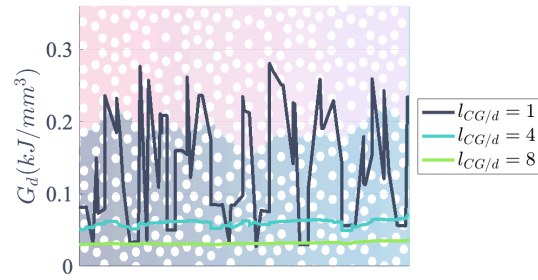
The average toughness G_d is inversely proportional to the coarse-graining scale l_{CG} (Figure 3.18(a)), and we find $G_d \sim \frac{1}{l_{CG}}$. Indeed, coarse-graining admits that the displacement, stress and strain fields on a material point actually depend on the state variables distribution in a neighbourhood of the point under consideration. The size of the neighbourhood is depicted by l_{CG} . To emphasize, we recall that all the results presented in this paper are found without any a priori on the material behaviour at the coarse-grained scales.

Remark 3.3. Here, we find $G_d \sim \frac{1}{l_{CG}}$ and $\sigma_f \sim \frac{1}{\sqrt{l_{CG}}}$. As previously stated, similar expressions relating the tensile strength σ_f (equivalently σ_c) to the characteristic length l_c , g_c and E can be found in [Nguyen et al., 2016, Benallal and Marigo, 2007, Pham et al., 2011b, Amor et al., 2009]. The expression derived from the uniaxial bar under traction with homogeneous damage distribution in Chapter 1 states $\sigma_c = \frac{9}{16} \sqrt{\frac{Eg_c}{3l_c}}$. This suggests that for a fixed toughness g_c (G_d), the same relation between σ_c and l_c (σ_f and l_{CG}) holds. However, we mention that no consensus on the relation linking E , σ_f , l_c and g_c taking into account the different loading conditions, and/or specimen geometries can be found in the literature. Further, we believe that the parametrisation of the elastic threshold in Chapter 1 may enable an additional degree of freedom in linking these quantities, and it may give the community the ability to incorporate geometric/loading factors within the framework without additional costs.

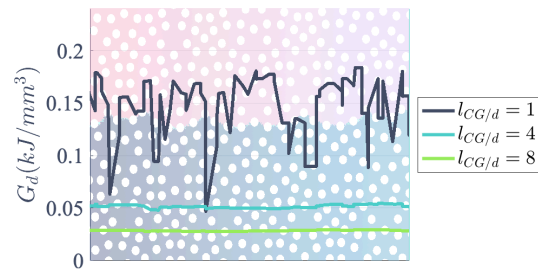
A study on the evolution of the 'homogeneity' of the effective toughness is conducted. In Figure 3.18, we plot the evolution of the effective fracture toughness G_d as a function



(a)



(b)



(c)

Figure 3.17 – Fracture toughness G_d evolution along the crack path for the Periodic (a), Quasi-Periodic type 1 (b) and Quasi-Periodic type 2 (c) microstructures.

of l_{CG} for the three microstructures (a) and the evolution of the corresponding coefficient of variation COV_{G_d} defining the heterogeneity of the effective toughness field (b).

As compared to the strength σ_f , one notices that the heterogeneity of the toughness field G_d is higher than the one of the strength field at the same scales. Yet no stability of the coefficient of variation of this quantity is observed at the large scales. As long as the crack path is straight, both the strength and the toughness evolve in the same manner at different coarse-graining scale. Regarding the Quasi-Periodic microstructures, one observes inversion of 'homogeneity' of the toughness in comparison with the strength, i.e., when comparing the plots in both Figure (a) and Figure (b), the blue and green curves corresponding to the coefficients of variation of σ_f and G_d are inverted; COV_{σ_f} is greater for the Quasi-Periodic type 2 microstructure as compared to Quasi-Periodic type 1, while COV_{G_d} is smaller. In fact, the crack might deflect to maximize its energy dissipation. This raises questions on the drift from *LEFM* where the notions of critical stress intensity factors and the critical energy release rate are somehow two faces of the same coin. Again, *FFT* analysis transformed from the effective toughness deviation D_{G_d} is presented in Figure 3.19.

For all three microstructures, small wavelengths $\lambda/d \leq 3$ are smeared-out as the coarse-graining scale increases and more weight on the larger wavelengths is observed $\lambda/d \geq 10$. In comparison with the strength responses, we can see that the larger wavelengths contributions to the heterogeneity of the toughness fields significantly increase as l_{CG} increases (a rise of more than 100%) for all the microstructures). The peak on $\lambda/d = 2 - 3$ observed at the smallest scale for the type 1 microstructure (in both the strength and the toughness responses) is decreasing as the coarse-graining increases to give way to the larger wavelengths (see Figure 3.19). As compared to the *FFT* analysis of the fracture strength, the dominant peaks observed at smaller scales are no longer present through the observation scales and this suggests the following: as the regularization via coarse-graining increases, the influence of the microstructure on G_d is smeared-out and the local phenomena intervening in the energy dissipation process are smoothed, which can lead to an actual homogenisation of this parameter in comparison with the strength σ_f where the microstructural influence persists even for larger coarse-graining scales.

§ 3.1. On the mesoscopic energy dissipation

The total dissipated energy W_d due to crack propagation can be computed following:

$$W_d(l_{CG}) = \int_{\Omega^0} G d\Omega, \quad (3.4)$$

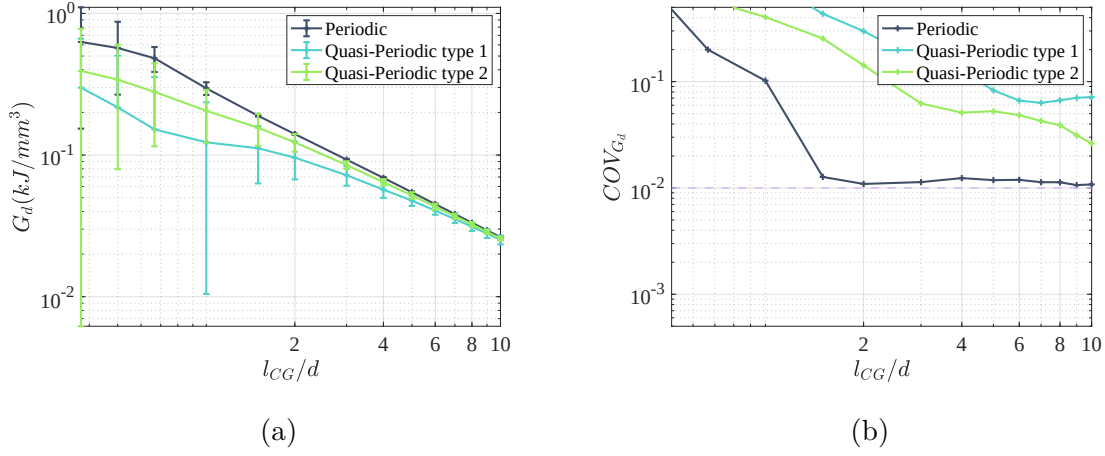
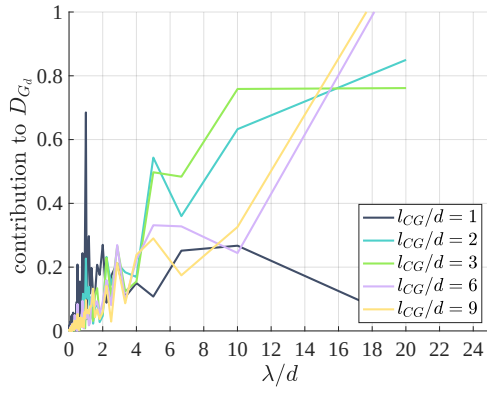
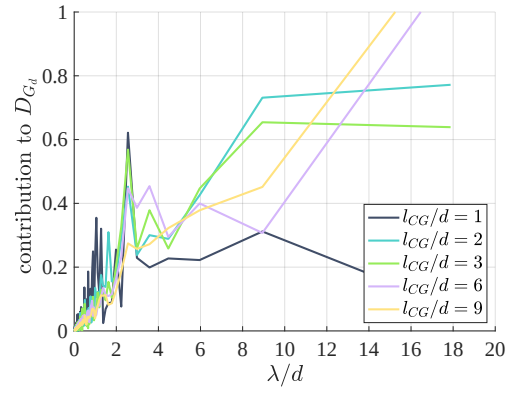


Figure 3.18 – Evolution of the effective fracture toughness G_d as a function of l_{CG} for the three microstructures (a) and the evolution of the corresponding coefficient of variation COV_{G_d} defining the heterogeneity of the effective fracture toughness field of the continuum (b)

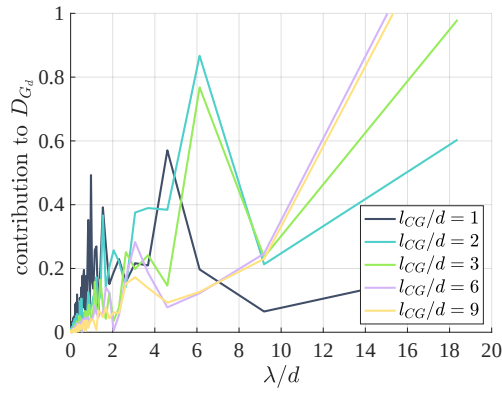
where G is the energy to total failure evaluated at each point in Ω^0 computed from $G = \int_0^{t_f} \mathbf{S} : \dot{\mathbf{E}} dt$. W_d thus corresponds to a measure of the energy dissipated in the coarse-graining volume (per unit thickness). Figure 3.20 shows the evolution of the total dissipated energy W_d for the different microstructures across the different mesoscopic scales l_{CG} . The dissipation is unsurprisingly conserved through the different mesoscopic scales. Even though G_d was found to be inversely proportional to l_{CG} (computed at the material points along the crack path), it's clear that the diffusion of damage on a larger zone thanks to the coarse-graining counterweights the decrease in G_d along the crack and conserves the overall dissipated energy across the scales. Unsurprisingly, the energy dissipation computed from the macroscopic (load-displacement) responses (Table 3.2) and the mesoscopic dissipations herein computed are equivalent, as the coarse-graining technique is based on the inviolable conservation laws.



(a)



(b)



(c)

Figure 3.19 – FFT analysis on the fracture toughness G_d for the Periodic microstructure (a), Quasi-Periodic type 1 (b) and Quasi-Periodic type 2 (c) microstructures.

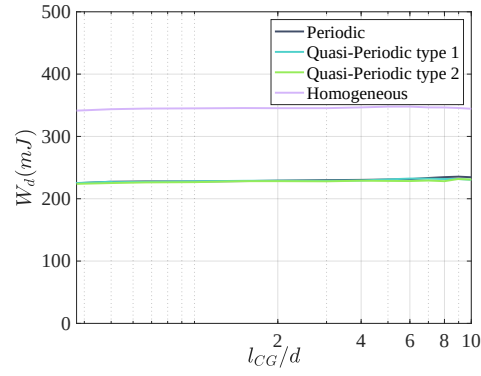


Figure 3.20 – Mesoscopic energy dissipation W_d , conservation of W_d is noted accross the scales and is equivalent to the energy dissipation computed from the load-displacement curve reported in Table 3.2

3.8 Concluding Remarks

In this chapter, we tackled the first of the three main branches of this thesis: the quasi-static crack propagation in architected materials, analysed at multiple scales. Phase-field simulation (Chapter 1) of failure on three architectures was considered for the micromechanical simulations. The obtained data are upscaled at different mesoscopic scales l_{CG} via the proposed coarse-graining technique (Chapter 2). Density, displacement, stresses and strain fields at the mesoscopic scales are constructed and analysis on the established database is lead. We summarise the main findings from this analysis:

Elastic properties From the micromechanical simulations before failure, coarse-grained elastic stresses and strains allow the computation of elasticity fields. Although the anisotropy of a microstructure is depicted by its symmetry order, the proposed scheme shows that a relatively large observation scale is needed for the symmetry order to reveal its influence. From the scale $l_{CG}/d = 1$, isotropic behaviour is obtained for the Periodic microstructure while the isotropy of the Quasi-Periodic structure requires $l_{CG}/d = 3$. The heterogeneities found at the microscopic scale influence the equivalent elastic properties at the mesoscopic scale. We show that in order to consider a homogeneous isotropic elastic equivalent medium, the required l_{CG} exceeds the values considered in the literature and in fact is much larger when considering non-periodic microstructures with long-range heterogeneities. For the Periodic distribution, an equivalent isotropic homogeneous elastic medium is found starting $l_{CG}/d = 1.5$, while for both Quasi-Periodic distributions, an $l_{CG}/d = 7$ is required to obtain an equivalent elastic homogeneous medium.

Crack propagation At the microstructural level, we show the presence of a preferential weak plane for propagation in the Periodic microstructure (similar to [Réthoré et al., 2017, Glacet, 2018]), and the presence of 'resilient zones' in the Quasi-Periodic material. As the crack gets trapped inside the holes, a much higher loading is required for the crack re-initiation, this phenomenon is mainly observed on the Quasi-Periodic microstructures. This phenomenon is reflected on the performances of each microstructure regarding the crack propagation.

The evolution of the crack paths shows prominent tortuosity across the observation scales. *FFT* analysis on the crack paths offers insight on the amplitudes and wavelengths that contribute to the effective crack paths deflections. For the type 1 Quasi-Periodic microstructure, peaks at similar wavelengths for different coarse-graining scales persist suggesting thus that the microstructural distribution of holes underlines the conservation

of the tortuosity and prohibits the consideration of a smooth effective failure band. For the type 2 microstructure, one clearly observes the absence of uniquely conserved high amplitude wavelengths across the scales which suggests a more readily smoothed crack path between the kinking spots.

Fracture strength The notion of strength emerging from the obtained coarse-grained stress-strain response was analysed. We define the fracture strength as the critical equivalent Rankine stress state reached at each effective crack tip position. The effective fracture strength is found to vary from one position of the crack tip to another along the crack path. This is explained by different phenomena including the trapping, re-nucleation, and deflection of the cracks after advancing inside the microstructure. This property is found to be the hardest to smear-out; in fact, the influence of the microstructure persists in all three microstructures even for relatively large coarse-graining scales. The stagnation of the coefficient of variation of the strength for the considered microstructures suggests the inability of the consideration of a homogeneous strength field for an effective medium that takes into account the heterogeneities at the smaller scales and that has a dominant role in stress concentration, crack initiation and general propagation. To better understand the microstructure's influence coupled with the scales, *FFT* of the crack paths and the fracture strengths are confronted. Even at large coarse-graining scales, i.e., where smoothing of local phenomena is expected, the strength remains highly influenced by the relatively small scales of the microstructures and large wavelengths do not have a significant influence on this quantity. This, with the evolution of the coefficient of variation of σ_f leads to believe in the impossibility to completely smear-out the heterogeneities involved in the fracture strength field of locally heterogeneous material.

Fracture Toughness We also propose a definition of the fracture toughness. Following the evolution of the coefficient of variation for the different microstructures, coarse-graining shows good ability to smear-out the microstructural effects on the equivalent toughness with no stagnation of the coefficient of variation at the large scales. *FFT* analysis of the fracture toughness evolution in the domain shows the large wavelengths contributions suggesting more easily smoothed parameter in comparison with the fracture strength, whereas the small wavelength amplitudes related to the microstructures are smeared-out.

This leads us to believe that considering a homogeneous model for simulating quasi-brittle failure in highly heterogeneous materials requires the consideration of extremely large scales to always be on the safe side when considering equivalent isotropic homogeneous

properties. We also show the inevitability of the consideration of a non-homogeneous material in which the influence of substructures is preserved at the mesoscopic scales.

Open issues and extensions The examples presented herein are limited to quasi-static crack propagation with imposed displacement. The absence of branching and multi cracks limited the analysis to a single crack propagation.

The consideration of the phase-field model at the microscopic scale to build the ground for the multi-scale analysis presented some limitations, especially regarding the calculation times. The arbitrary mesoscopic discretization choice H did not influence on the overall results and only alters the resolution of the coarse-grained fields. The maximum observation scale l_{CG} is bounded by the size of the considered TDCB geometry.

DAMPING PROPERTIES OF PERIODIC AND QUASI-PERIODIC ARCHITECTURED MATERIALS

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4.1 Introduction

In the previous chapter, the quasi-static failure of the architectures shows interactions between the crack and the microstructures. Since the crack tends to follow the path that would allow maximum energy dissipation, it's found that the crack avoids 'resilient patterns' in the Quasi-Periodic material and follows 'weak' planes in the Periodic material.

When moving to dynamic fracture, a new player enters the game: the stress waves. **How?** Any applied loading will induce disequilibrium of the medium, which induces the

different portions of a material to move and adjust towards their equilibrium state, this adjustment propagates from the loading application towards the bulk, this phenomenon constitutes the general basis of 'stress-wave propagation'.

At low strain-rates, the adjustment 'has sufficient time' to attain equilibrium before any subsequent external change occurs, quasi-static conditions may apply. At high strain-rates, there isn't sufficient time for stress equilibrium to be achieved before subsequent changes, so the analysis of the inertial effects is prominent, and the stress-wave propagation must be followed.

In recent years, architected materials have attracted increasing attention among the scientific community due to their extraordinary acoustic and elastic wave propagation performances. In fact, after the wide studies regarding the atomic dynamics, photonic, magnetic, electronic wave propagation and band-gaps properties in Quasi-Periodic materials, efforts were undertaken to transport these features to larger scale architected materials.

Understanding the attenuation of stress-waves in model Periodic and Quasi-Periodic architected materials is sought in this chapter.

To study the influence of the microstructure on stress-wave propagation and dynamic properties of the architected materials (the Periodic and Quasi-Periodic type 1 & 2), 2D finite element (FE) simulations are performed on out-of-equilibrium stress-wave packet propagation. A direct comparison is established between the Periodic and Quasi-Periodic microstructures vis-à-vis their acoustic (stress-wave propagation) and effective behaviour.

The chapter is organized as follows: first, the numerical tools required for the analysis are advanced: the rectangular sample embedding the architectures and the boundary conditions are presented; stress-wave packets of different wave-lengths are followed along the samples embedding the architectures. From here, different points are tackled: (i) the kinetic energy envelope and the penetration lengths are studied and related to the attenuation performances; (ii) the effective (long-wavelength) and instantaneous stress-wave speeds are estimated and related to the transportation regimes; (iii) the transition from propagative to diffusive regimes with increasing excitation wavelengths is tackled; (iv) *FFT* analysis on the velocity at the outlet of the microstructure to offer insights on the amplitudes and wavelengths that are passed/rejected by the microstructure.

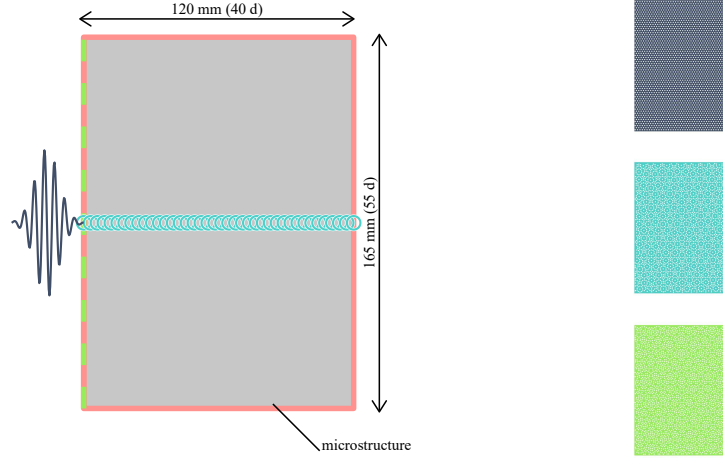


Figure 4.1 – Imposed wave-packet on the left boundary of the sample (green-dashes). Silent Boundary Conditions (SBC) are set on the four boundaries (orange), the effective attenuation is studied along the x – direction of the blue frames. At the right-hand side of the figure are represented the three architectures

4.2 Numerical tools

4.2.1 Architected sample

FE simulations are considered for the study of vibrational properties of the typical microstructures (Section 0.4, Figure 8, Table 1). The samples are of a simple rectangular shape of dimensions $55d \times 40d$. The microstructures are embedded by bulk material zones of width $0.5d$ as shown in Figure 4.1. The wave-packet is generated by imposing a velocity on the left side following the work in [Luo et al., 2021]:

$$V(\lambda_{in}, t) = V_0 \exp\left(-\frac{(t - 3t_0)^2}{2t_0^2}\right) \sin\left(2\pi \frac{c_d}{\lambda_{in}} t\right) \quad (4.1)$$

V_0 is a constant value, ω_{in} is the frequency of the quasi-monochromatic excitation and relates to the wavelength λ_{in} of the wave-packet via the stress-wave speed $\omega_{in} = (2\pi \frac{c_d}{\lambda_{in}})$, and $t_0 = \frac{3\pi}{\omega_{in}}$ is the half period of the excitation.

4.2.2 Longitudinal wave-packet excitation

Excitation perpendicular to the boundary corresponds to a longitudinal one while the imposed velocity parallel to the boundary corresponds to a transverse excitation. Here,

the focus is shed on the longitudinal wave propagation imposed at the left-hand boundary of the specimen. It's noted that the remaining boundaries are set to Silent Boundary Conditions (SBC). Technical details about the SBC can be found in [Rossmanith, 2002]. The application of (SBC) reduces unwanted reflections that may affect the analysis by mimicking an infinite medium. Once the full wave-packet is imposed, the left boundary is also set to a non-reflective one (SBC). Of course, periodic boundary conditions could be considered for the analysis [Luo et al., 2021, Glacet, 2018, Glacet, 2019], for the Periodic microstructure, and for a periodic approximation of the Quasi-Periodic ones. However, as the approximation might induce some unwanted bias, the decision to consider the same numerical model for the different microstructures was carried-out. Regarding the material in question, it is linearly elastic with an isotropic homogeneous behaviour characterised by the typical mechanical properties presented in Table 4.1. Plane strains are assumed.

ρ	$1180kg/m^3$	c_d	$2278m/s$
E	$2.4GPa$	c_s	$846m/s$
ν	0.42	c_R	$800m/s$

Table 4.1 – Bulk material properties

ρ corresponds to the mass density, E and ν denote respectively Young's Modulus and Poisson ratio. c_d , c_s and c_R designate the longitudinal, shear and Rayleigh stress-wave speeds.

Transient simulations of wave propagation ($\lambda_{in} = d, \dots, 10d$) are conducted using explicit dynamic FEM. The time step is taken to be equal to $dt = 47ns$, smaller than the Courant time step (i.e., the time taken by a sound wave to travel across an element) for increased precision. The technical details about the time integration scheme can be found in [Sun et al., 2000].

4.3 Kinetic energy Envelope

As mentioned, the wave-packet is imposed on the left boundary of the sample. Its propagation inside the microstructure is then followed along the x -direction. As the wave-packet travels inside the sample, it's scattered due to the reflections on the free boundaries of the holes. To understand how such scattering affects the energy transfer, we compute the envelope of the kinetic energy P_m^K for each material point m at each input frequency

(ω_{in}) of the FE simulation set as:

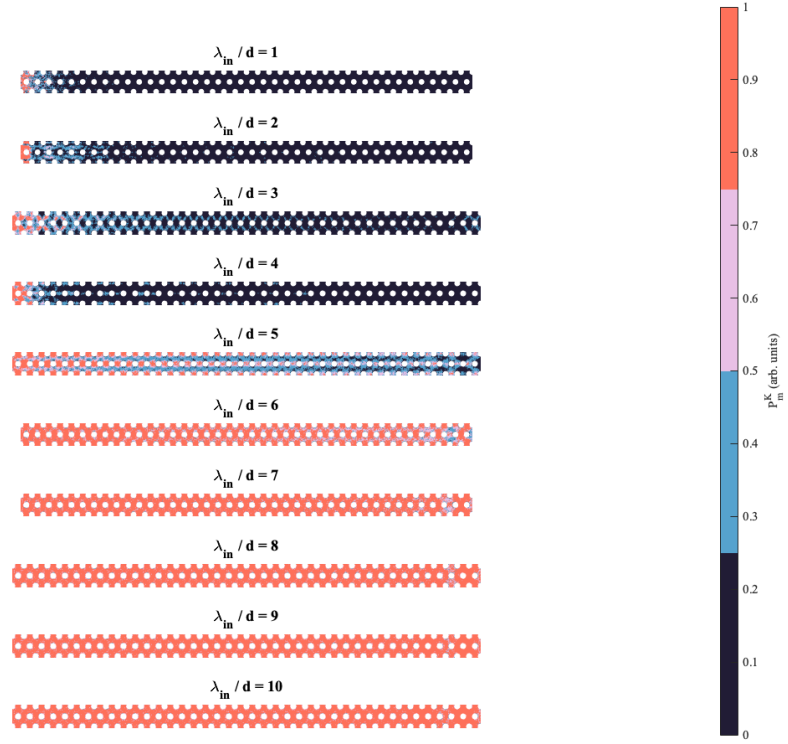
$$P_m^K(\omega_{in}) = \max_t K_m(\omega_{in}, t) \quad (4.2)$$

where $K_m(\omega_{in}, t)$ is the kinetic energy at material point m , for the simulation of the excitation of frequency ω_{in} at time t .

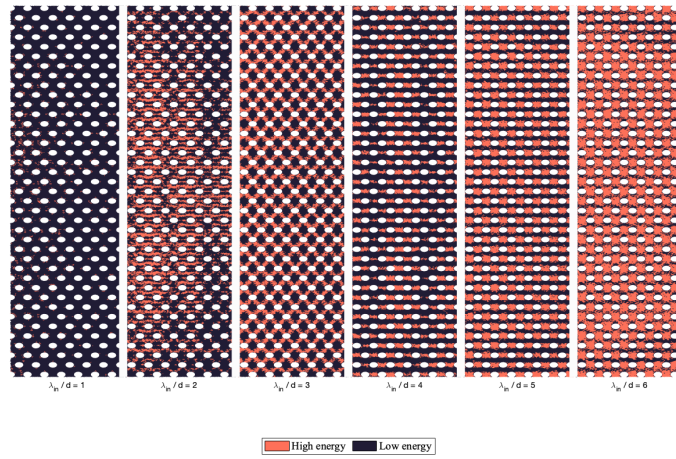
Figure 4.2 shows results of the attenuation of the kinetic energy at different λ_{in} for the Periodic microstructure. In Figure 4.2(a), the spatial attenuation of the kinetic energy at the middle of the sample along the x - direction (principal direction of stress-wave propagation) is showcased. It's mentioned that the energy is normalised by its value at the inlet (near the boundary on which the wave-packet is imposed). It's clear that the energy attenuation is much more pronounced at higher excitation frequencies (small wavelengths), and inversely, the wave-packet seems to be unaffected by the microstructure at excitation wavelengths larger than $\lambda_{in}/d = 5$. Surprisingly, at $\lambda_{in}/d = 3$, this trend is distorted, as the envelope shows higher energy as compared to envelope obtained at the larger $\lambda_{in}/d = 4$.

For a comprehensive analysis, a larger zone of the microstructure is put-forth in Figure 4.2(b), showing the envelope of the kinetic energy at some interesting wavelengths ($\lambda_{in} = d, \dots, 6d$), and separating the microstructure into zones of high/low kinetic energies. Here, the results are normalised by the mean value of the energy envelope inside the sample for better visualisation and to allow for a cleaner interpretation of the zones. Different energy patterns are present and it is clear that this is the result of different interactions between the wave-packet λ_{in} and the microstructural holes distribution. At small wavelengths, the energy is localised near the boundary on which the wave-packet is imposed. At $\lambda_{in} = 3d$, a special pattern of the energy envelope is observed, and this interaction between the periodic distribution of holes and the wavelength of the input wave-packet might explain the higher energy recovered at the right of the specimen at this frequency. At $\lambda_{in}/d = 4$ and $\lambda_{in}/d = 5$, the energy is localised along horizontal lines between the holes.

The same analysis is performed on the Quasi-Periodic microstructures (Figures 4.3 and 4.4). Differently from the Periodic type microstructure, no disturbance in the trend of the overall attenuation varying in opposition of the wavelength is observed. However, regarding the attenuation along the x - direction, It is clear that the envelope presents much more pronounced oscillations correlated with the presence of varying hole distribution, without any clear periodicity (as compared to the periodic patterns found in Figure 4.2(a)). In

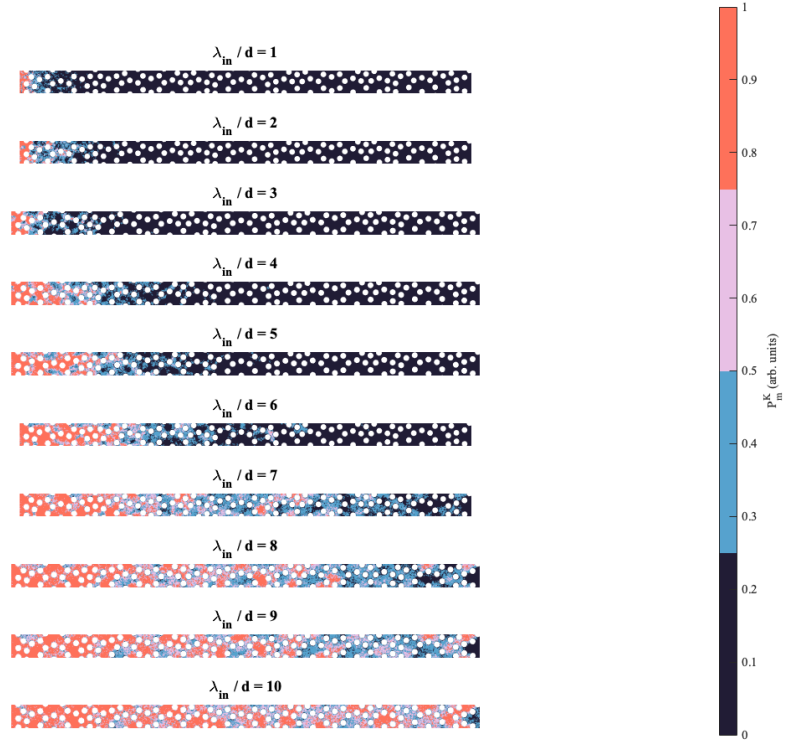


(a) Envelope of the attenuation of the kinetic energy

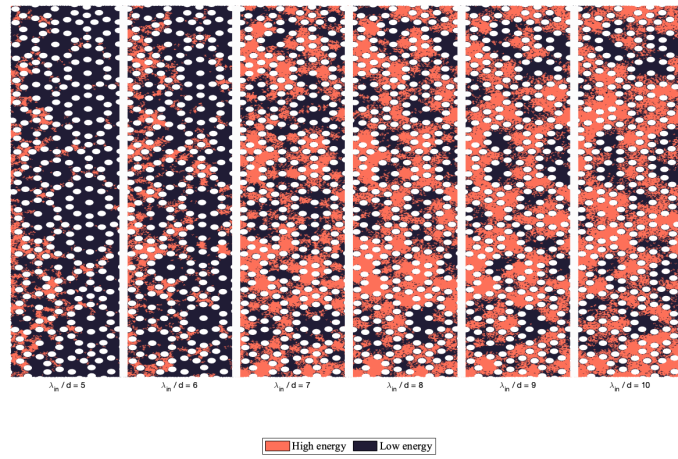


(b) Separation of the Periodic microstructure into zones of high/low kinetic energy envelopes for interesting λ_{in} values

Figure 4.2 – Envelope of the kinetic energy at different λ_{in} : interactions with the patterns of the Periodic microstructure

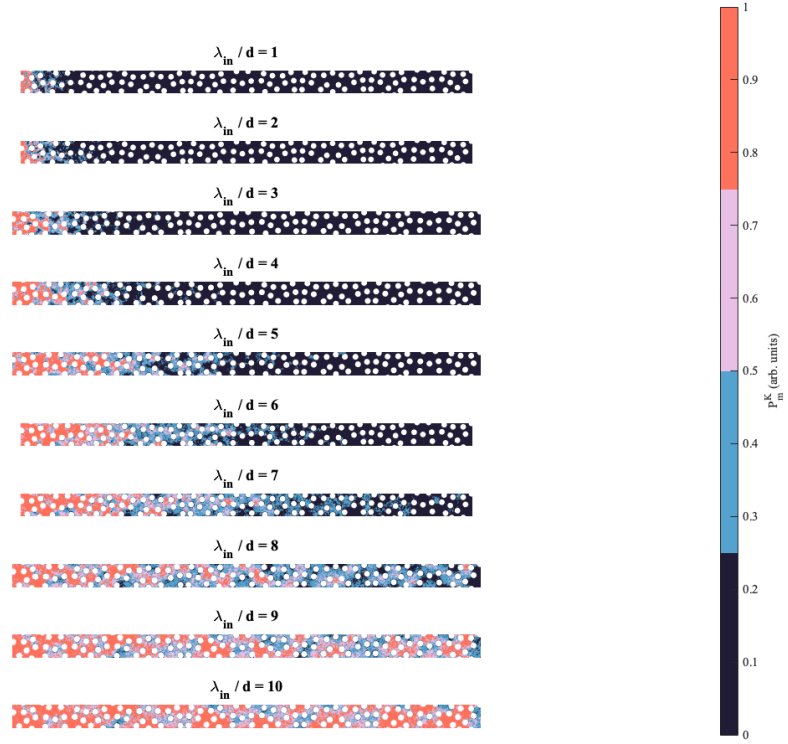


(a) Envelope of the attenuation of the kinetic energy

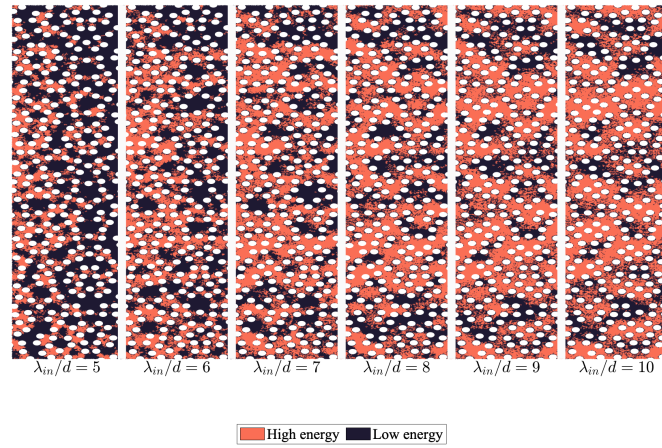


(b) Separation of the Quasi-Periodic type 1 into zones of high/low kinetic energy envelopes for interesting λ_{in} values

Figure 4.3 – Envelope of the kinetic energy at different λ_{in} : interactions with the patterns of the Quasi-Periodic type 1 microstructure



(a) Envelope of the attenuation of the kinetic energy



(b) Separation of the Quasi-Periodic type 2 into zones of high/low kinetic energy envelopes for interesting λ_{in} values

Figure 4.4 – Envelope of the kinetic energy at different λ_{in} : interactions with the patterns of the Quasi-Periodic type 2 microstructure

the previous Chapter 3, studies on this typical microstructures in quasi-static simulations of failure show the presence of what is known as "resilient patterns", i.e., zones in the Quasi-Periodic distribution around which the crack always deviates and rarely travels through (refer to Section 3.5 to recall the influence of these zones on the quasi-static crack propagation). As seen in Figure 4.3(b), the energy envelope inside those typical patterns are in the low-energy zones even at the largest wavelengths $\lambda_{in} = 5d, \dots 10d$. We recall that these maps actually represent a spatial distribution of the maximum kinetic energy 'viewed' by each material point in time, so these low energy-zones prohibit the passage of the wave-packet within. In the case of the Quasi-Periodic type 2 microstructure (Figure 4.4), similar influence on the energy attenuation is observed as for the type 1 microstructure, moreover, the presence of "resilient patterns" is noted across the studied range of wavelengths (Figure 4.4(b)). The Quasi-Periodic microstructures appear as more efficient for energy attenuation; intuitively, one might suggest more efficient scattering around these "resilient patterns". Further on this point is to be found in the following sections.

4.4 Energy Attenuation and penetration length

Since the FE simulations are performed at constant energy (no damping - except at the silent non-reflective boundaries SBC, that are far enough from the region of interest and that do not affect the analysis), the attenuation in the energy envelope actually comes from the redistribution of the kinetic energy in directions different than the principal direction of propagation (namely the x - direction). This is a direct result of the scattering of the wave-packet that happens at the interfaces of the microstructures. The effective attenuation along the x -direction is studied by following energy transport at the middle of the sample at $x = x_f$ in consecutive frames of width $l_{CG} = d$ (Figure 4.1)):

$$P^K(\omega_{in}, x_f) = \max_t K(\omega_{in}, x_f, t) \quad (4.3)$$

Where $K(x_f, t)$ is the kinetic energy supported by the frame located at $x = x_f$ of width $l_{CG} = d$ at time t . Figure 4.5 shows a comparison of the envelopes between the three microstructures at different excitation frequencies. Figures 4.5(a), 4.5(b) and 4.5(c) show the envelope of the kinetic energy at different λ_{in} related to the characteristic length d of the Periodic, Quasi-Periodic type 1 and 2 microstructures respectively. Due to the effective

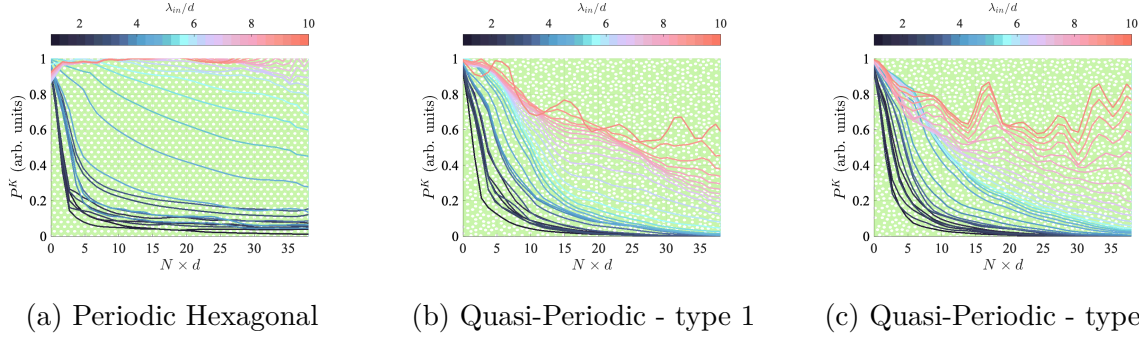


Figure 4.5 – Comparison of the kinetic energy envelopes P^K in the three microstructures along the middle of the samples

rigidity contrast at the right and left boundaries of the microstructure (due to the presence of a full-band of width $0.5d$), the attenuation analysis is started at the position of the first holes and ended at $x_f = 38d$.

For the Periodic microstructure, at least half of the energy is transported throughout the sample when the excitation wavelengths exceed 5 times the characteristic length d of the microstructure. At smaller wavelengths, scattering of the stress waves strongly attenuates the wave-packet. In the studied range of small wavelengths, the energy fails to travel across the sample, e.g., at $\lambda_{in} = d$, $P^K \leq 0.01$ at the outlet. A peak in the transported energy at $\lambda_{in} = 3d$ is noted, meeting well with previous observations on the special energy envelope patterns found at this frequency. For the Quasi-Periodic microstructures, oscillations in the energy envelope are observed. As mentioned previously, this notable oscillation (as compared to results on the Periodic microstructures) is a direct result of the "resilient patterns" inside this type of microstructures. No energy transport across the microstructure is observed at excitation wavelengths $\lambda_{in} \leq 5d$, where ($P^K \leq 0.01$ at the outlet). Even for larger λ_{in} , the entirety of the wave-packet could not be totally recovered at the right boundary of the sample. The long-range pattern heterogeneities in the Quasi-Periodic materials could provide continuous source of scattering leading to more efficient kinetic energy attenuation.

As seen, for the considered sample geometry and microstructural holes distribution, the strength of the attenuation inside the architecture depends on two main parameters: the wave-packet frequency and the hole distribution. For instance, in case of large wavelengths, the attenuation is similar to a Beer-Lambert law [Beltukov et al., 2018, Swinehart, 1962] (see Figure 4.6 for a schematic of the law, using arbitrary units), where the envelope of

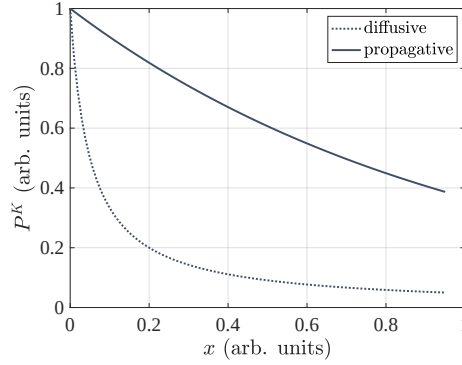


Figure 4.6 – Schematic of propagative and diffusive energy transportation regimes following the Beer-Lambert and Gaussian law with arbitrary units, displayed for a qualitative comparison of the simulation results

the energy transportation is written:

$$P^{prop,K}(\omega_{in}, x_f) = \frac{\epsilon_0(\omega_{in})}{\pi v^2 \tau_{exc}^2} e^{-x_f/l} \quad (4.4)$$

with a mean free path l , $\epsilon_0(\omega_{in})$ being the total kinetic energy introduced to the sample from external excitations of duration τ_{exc} and v corresponding to the stress-wave speed c_s or c_d). The maximum kinetic energy moves (left to right) and gradually decreases due to the scattering by the structural disorder (Figure 4.6). This is a typical signature of a propagative regime [Beltukov et al., 2018].

In the case of small wavelengths, the kinetic energy envelopes read:

$$P^{diff,K}(\omega_{in}, x_f) = \frac{\epsilon_0(\omega_{in})}{2\pi e} \frac{1}{x_f} \quad (4.5)$$

which is a signature of a diffusive process [Beltukov et al., 2018]. The maximum of the kinetic energy decays exponentially (Figure 4.6).

By qualitatively analysing the trends of the kinetic envelopes, one observes pinning of the wave-packet at the inlet of the microstructure (left) at small wavelengths. By fitting the envelopes (Figure 4.5) to the Equations 4.4 and 4.5, insights on the dominant transportation regime in each architecture at each λ_{in} is obtained. As the wavelength increases, the transition occurs smoothly for the Periodic microstructure at intermediate wavelengths $4 < \lambda_{in}/d \leq 5$. At larger wavelengths, the propagative regime appears dominant until minor to no attenuations are reached at largest studied wavelengths. At

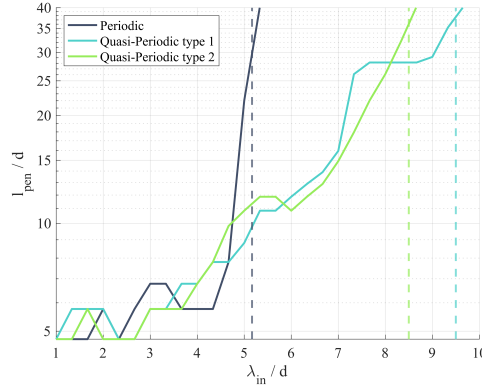


Figure 4.7 – Penetration length l_{pen} for the smoothened kinetic energy envelopes for the three microstructures

the special wavelength $\lambda_{in} = 3d$, propagative regime is predominant.

For the Quasi-Periodic materials, the transition appears much later, around $6 < \lambda_{in}/d \leq 7$ for the type 1 and type 2 microstructures.

After comparing the kinetic energy envelopes of the three microstructures at different wavelengths and observing the sound interactions between the wave-packet and the microstructures, the attenuation is now quantified by investigating the long-time penetration length. The penetration length l_{pen} is defined as the distance above which the kinetic energy stays below the maximum excitation kinetic energy, i.e., provided energy at the boundary, divided by e (Euler's number): $P_{l_{pen}}^K(\omega_{in}) = \frac{1}{e} P_0^K(\omega_{in})$. Figure 4.7 reports the penetration-lengths for the three architectures at different excitation wavelengths. The dashed-lines correspond to the wavelengths from which the kinetic energy is no more attenuated below the $(1/e)$ threshold of its initial value. At the smallest wavelengths, the Periodic microstructure shows better performance in attenuating the wave-packet. At the special wavelength $\lambda_{in} = 3d$, a local maximum of the penetration length in the Periodic material is observed mirroring previous results; here the Quasi-Periodic architectures show a better performance in attenuating this wavelength. Around, $\lambda_{in}/d = 4$, the more efficient attenuation of the Periodic microstructures are recovered. But from $\lambda_{in}/d \simeq 5$, no attenuation below $\frac{1}{e} P_0^K(\omega_{in})$ is observed in the Periodic architecture.

In the Quasi-Periodic microstructures, the penetration lengths increase gradually with the wavelengths suggesting an improved efficiency in attenuating the wave-packet starting $\lambda_{in}/d = 5$ over the Periodic microstructures, and of course, earlier at $\lambda_{in}/d = 3$.

4.5 Sound velocity

After qualitatively analysing the different regimes of energy transport in the specific range of wavelengths, the effect of the diffusive contribution to the energy transport is investigated via an analysis on the stress-wave speeds. In highly heterogeneous linearly elastic materials, wave-propagation is mainly influenced by two factors, the effective rigidity of the medium (i) and the interfaces features at the heterogeneities(ii) [Luo et al., 2021]. Indeed, as the wave-packet travels inside the microstructure, its scattering leads to a redistribution of the kinetic energy in directions different than the principal direction of propagation changing thus the apparent wave-packet speed.

First, the effective wave-speed at larger wavelength is determined (i), then, the instantaneous waves-speeds reported at different positions of the wave-packet average position are computed (ii).

4.5.1 Long-wavelength (effective) velocity

To estimate the effective wave-speed at large wavelength, the effective elasticity moduli and density are computed following the coarse-graining method suggested in Chapter 2. In Chapter 3, we showed the ease of convergence towards a mean (converged) effective isotropic elasticity tensor from relatively small coarse-graining scales. Table 4.2 summarizes the effective material properties, namely the effective density and elastic properties of the Periodic and Quasi-Periodic types 1 and 2 microstructures, along with the bulk (homogeneous) material properties (as seen in Table 1). The effective longitudinal wave-speed is then computed for each microstructure from their corresponding effective converged material properties.

However, this calculation cannot transcribe the diversity of behaviour of the stress waves in the highly heterogeneous microstructures in transient state, i.e., energy redistribution. In consequence, the instantaneous speed of the wave-packet must be studied. This should give more insights on the transient properties of the architectures.

4.5.2 Instantaneous velocity

The different patterns and heterogeneities' distribution suggest a big impact on the stress-wave propagation - as seen in the previous sections. At wavelengths comparable to the microstructures' characteristic length(s), this influence is most pronounced and

Typical microstructures effective properties				
Geometry	Young Modulus (GPa)	Poisson ratio	density (kg/m ³)	c_{def} (m/s)
Bulk	2.400	0.420	1180	2279
Periodic	1.395	0.354	931	1563
Quasi-Periodic type 1	1.244	0.348	892	1489
Quasi-Periodic type 2	1.220	0.354	892	1495

Table 4.2 – Elasticity moduli, density and the longitudinal wave-speed for the bulk material. Effective elasticity moduli, density and the long-wavelength (effective) speed for the Periodic and Quasi-Periodic type 1 and 2 microstructures, computed at scale $l_{CG} = 10d$ (converged moduli following Chapter 2 and 3), plane strains are assumed

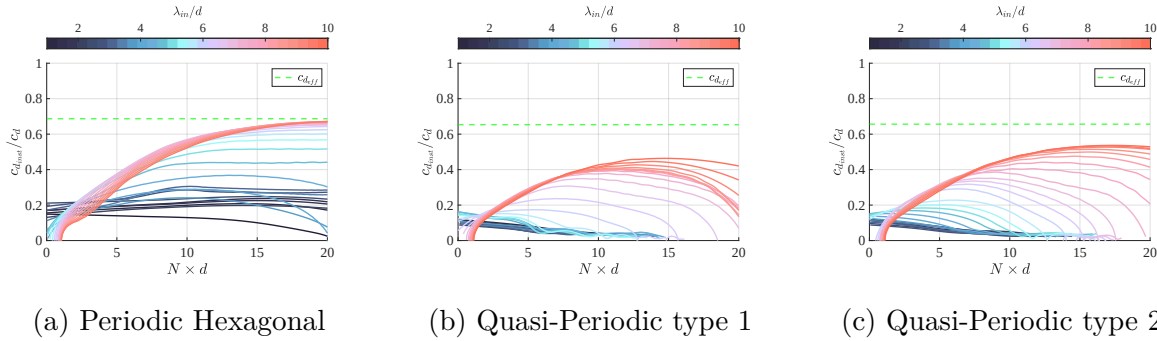


Figure 4.8 – Evolution of the instantaneous wave-packet speed in the microstructure.

the stress-waves scattering is accompanied by an attenuation of the wave-packet speed as it travels different zones in the microstructure. To further quantify this scattering and attenuation, the instantaneous wave-speed is assessed. The instantaneous wave speed reported at each position of the wave-packet inside the microstructure is computed as follows [Luo et al., 2021, Luo et al., 2019]:

$$\begin{aligned}
 x_w(\omega_{in}, t) &= \frac{\sum_m x_m K_m(\omega_{in}, t)}{\sum_m K_m(\omega_{in}, t)} \\
 c_{d_{inst}}(\omega_{in}, t) &= \frac{\partial x_w(\omega_{in}, t)}{\partial t}
 \end{aligned} \tag{4.6}$$

Due to scattering, the energy transport is not monotonous and the energy is expected to bounce back and forth as the stress-waves are scattered inside the microstructures between the holes patterns. Consequently, the instantaneous velocity, especially of the wave-packets of small wave-lengths, ricochets from negative to positive values and vice-versa; hence the need to smoothen the obtained values of $x_w(\omega_{in}, t)$ and $c_{d_{inst}}(\omega_{in}, t)$. A Savitzky-Golay filter is considered.

Figure 4.8 shows the evolution of the instantaneous wave-speed in the three considered microstructures as the wave-packet travels inside the sample for different excitation wavelengths. As the wave-packet is establishing in the sample, we note an initial speed rise time (mainly visible at large-wavelengths wave-packets). Only the velocity values after this initial increase should be considered for the analysis. Moreover, the silent boundary condition at the right of the sample reduces the zone in which the instantaneous velocity estimation is lucid. In fact, the wave-packet approaches the right boundary of the sample, it's absorbed by the imposed silent boundary condition and thus the computation of x_w following Eq. 4.6 becomes erroneous (mainly at large-wavelengths). Hence the reduction of the studied zone width to $20d$ (instead of $40d$) corresponding to a width of $60mm$ (instead of $120mm$).

As shown, with increased λ_{in} , the value of the established instantaneous velocity increases.

This is especially true for the Periodic microstructure where a typical convergence towards the effective value found in Section 4.5.1 suggests a clear establishment of the wave-packet inside the architecture with minimal scattering. The absence of a plateau at the smallest wavelength $\lambda_{in}/d = 1$ is a signature of a diffusive-localized regime in total agreement with the penetration lengths reported previously. From $\lambda_{in}/d = 4$, one observes a plateau in the instantaneous velocity suggesting thus the dominance of the propagative regime of the energy transport [Luo et al., 2021]. At the special wavelength of $\lambda_{in} = 3d$, we can see a peak in the instantaneous velocity mirroring the previous results on the Periodic microstructure at this specific excitation frequency. It's mentioned that these results are in accordance with the penetration length results reported in Figure 4.7.

For the Quasi-Periodic microstructures, the instantaneous speed is always lower than the estimated long-wavelength values reported in Table 4.1. This indicates a persistent attenuation of the energy transport in total agreement with the penetration lengths analysis reported previously. It's noted that the Quasi-Periodic type 1 microstructure appears to be the most efficient in scattering the wave-packet from this interpretation on the instantaneous wave-speeds; a result observed in Section 4.3. The instantaneous speed in the Periodic architecture is found to be systematically larger than the one in the Quasi-Periodic architectures, showcasing the higher efficiency of the Quasi-Periodic microstructures in slowing down and reducing energy transport.

In the next section, we follow [Beltukov et al., 2018] and proceed to analyse the transition from propagative to diffusive regime.

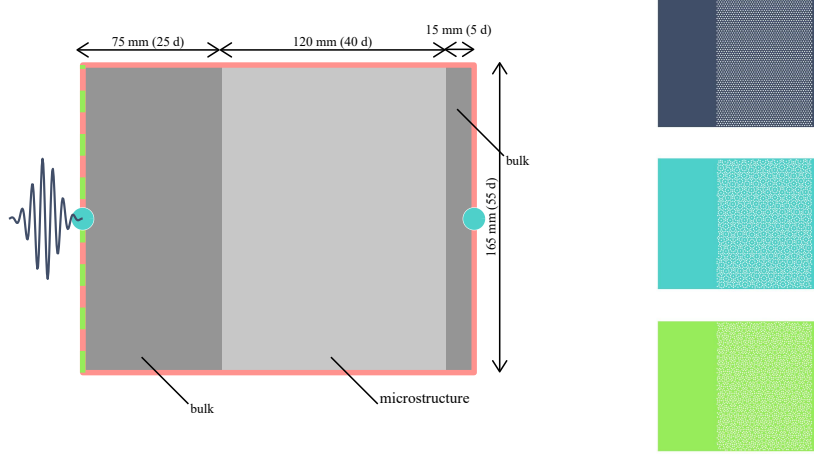


Figure 4.9 – Microstructure at the core of the sample considered for the analysis of the input(left)/output(right) (blue dots) wave-packet. Imposed wave-packet on the left boundary of the sample (green-dashes). Silent Boundary Conditions (SBC) are set on the four boundaries (orange). At the right-hand side of the figure are represented the three architectures

4.6 From propagative and diffusive regimes

For a given position m , the kinetic energy evolution in time $K^m(\omega_{in}, t)$ gives insights either on the coexistence of propagative and diffusive energy transfer, or the dominance of one over the other. The analytical method proposed by [Beltukov et al., 2018] is followed to analyse the transportation of energy. For this, we consider the microstructure ($40d \times 55d$) embedded at the core of a rectangular sample of $70d \times 55d$ (Figure 4.9).

This allows the analysis of (i) the input signal (wave-packet) with no reflection/scattering from the microstructures at the left of the sample, and of (ii) the wave-packet at the outlet (right) as the wave travels across the sample (Figure 4.9). The input and output wave-packet will subsequently be analysed in the frequency domain to offer insights on the amplitudes and wavelengths that are passed/rejected by the microstructure (Section 4.7).

Figure 4.10 shows the time evolution of the kinetic energy K_{out} at the outlet (vibrant colours) and K_{in} at the inlet (faded colours) of the three microstructures for three excitation wavelengths. The upper envelope (thick lines) is considered here for the analysis. It's noted that for each i -wavelength, the plots were rescaled by i^{-3} and normalised by their corresponding maxima for a better visualisation. The focus is shed on K_{out} . For the three microstructures, most prominently at large wavelengths, a narrow peak PK_{out}^{prop} is observed at first (at time $t = t_{out}^0$), followed by a broader peak PK_{out}^{diff} (or multiple

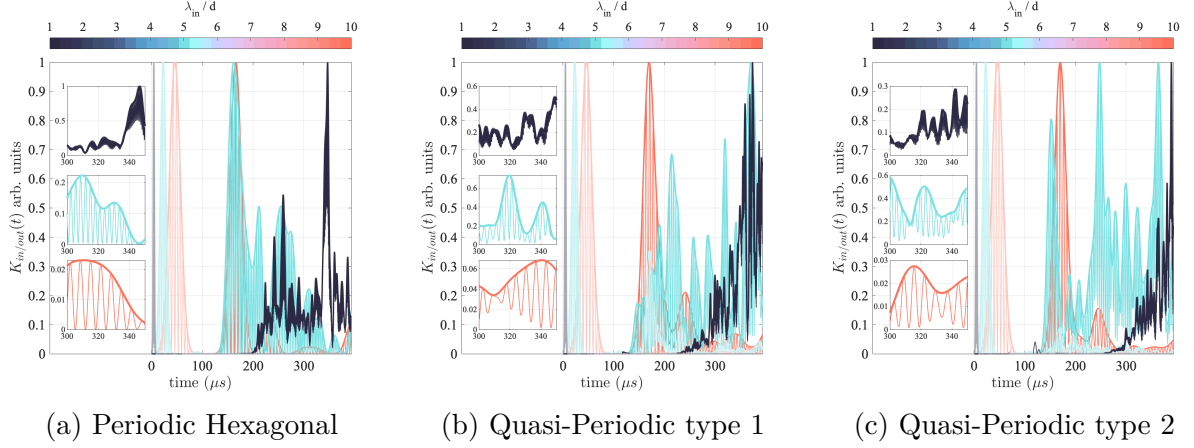
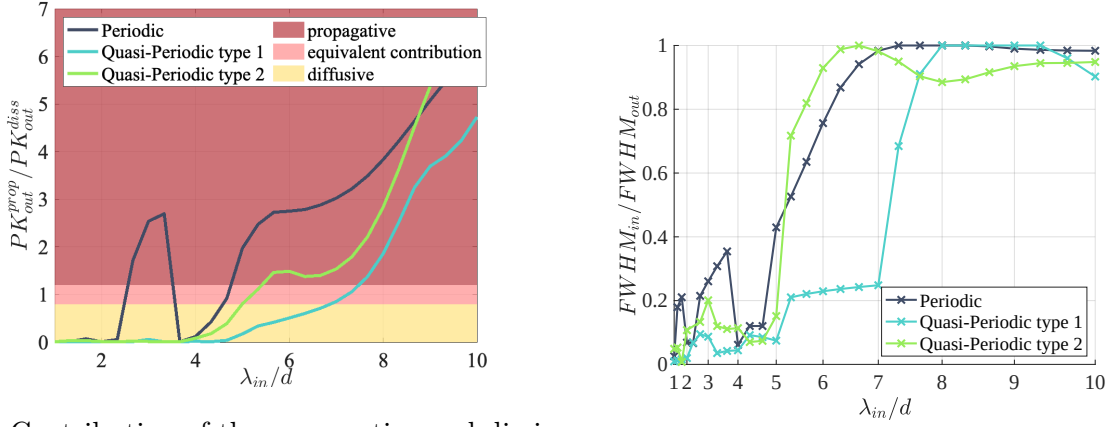


Figure 4.10 – Time evolution of the kinetic energy at the outlet (vibrant colours) K_{out} and the inlet K_{in} (faded colours) of the microstructures, each one is normalised for visualisation purposes. Three wavelengths are represented. The upper envelope (thick lines) is considered for both the PK and $FWHM$ analysis.

superposing peaks) of the energy. As mentioned in previous works [Beltukov et al., 2018], the first peak in the kinetic energy corresponds to the so-called propagative peak; the following peak(s) is(are) formed by the diffusive spreading of the scattered energy and is(are) known as the diffusive peak(s). From Figure 4.10, the propagative peak is shown to be very different for each microstructure, and especially at intermediate wavelengths (e.g., $\lambda_{in}/d = 5$). For small wavelengths, there's no clear and distinguishable propagative peak: the diffusive energy transfer regime is predominant. As the regime shifts from a diffusive to propagative one with increasing λ_{in} , the contribution of the propagative peak increases; the contribution of the diffusive peak is in its turn reduced. Following [Beltukov et al., 2018], the ratio between the propagative peak (PK_{out}^{prop} at $t = t_{out}^0$) to the diffusive peak (PK_{out}^{diff} at $t > t_{out}^0$) can be used as a criterion to identify the dominant regime of energy transfer at each λ_{in} for each microstructure. We recall that the herein shown peaks cannot represent by any mean any sort of attenuation between the inlet and outlet since each plot is normalised by its own maxima for visualisation purposes, as we focus solely on the kinetic energy at the outlet, and we analyse its trends.

The evolution of the peaks ratio $\frac{PK_{out}^{prop}}{PK_{out}^{diff}}$ (propagative to diffusive) with the excitation wavelength λ_{in} is plotted in Figure 4.11(a) for the three microstructures. The transition from diffusive to propagative regime occurs for the Quasi-Periodic type 1 and 2 at $\lambda_{in}/d = 7$ and $\lambda_{in}/d = 5$ respectively. For the Periodic microstructure, around the special



(a) Contribution of the propagative and dissipative peaks to the kinetic energy at the outlet of the microstructures.

(b) $FWHM$ of the kinetic energy at the outlet suggesting transfer regime transition

Figure 4.11 – Analysis of the transition from propagative (low-frequency, large wavelength) to dissipative (high-frequency, small wavelength) regime.

wavelength of $\lambda_{in} = 3d$, a peak in the ratio suggests a dominant propagative regime. From $\lambda_{in}/d = 5$, only propagative regime is observed. At large wavelengths, namely $\lambda_{in}/d \geq 5$, the propagative regime is predominant in the three microstructures, and this dominance is mostly pronounced in the Periodic microstructure.

A comparison of the width of the signal, computed as the full width at half maximum $FWHM$ of the energy packet at the outlet with the width of the excitation (the wave-packet at the inlet) also describes the effective diffusivity of the energy inside the microstructures. The broadening of the energy peak is signature of the diffusive transfer regime, while a constant width corresponds to a dominant propagative regime.

Figure 4.11 shows the evolution of the ratio between the inlet width of the wave-packet and the outlet width of the wave-packet $\frac{FWHM_{in}}{FWHM_{out}}$. An S shape trend is observed for the three microstructures. At high frequencies (small λ_{in}), the broadening of the wave-packet is the most pronounced for the three microstructures, thus the dominance of the dissipative regime. For the Periodic microstructure around $\lambda_{in}/d = 3$, a peak in the $FWHM$ ratio is observed suggesting a transition from dissipative to propagative regime. From $\lambda_{in}/d = 5$ to $\lambda_{in}/d = 7$, coexistence of both diffusive and propagative regimes is proposed. For the Quasi-Periodic type 1 microstructure, no widening of the wave-packet occurs starting $\lambda_{in}/d = 8$, for wavelengths $\lambda_{in}/d \leq 7$, dominance of the diffusive transportation regime is observed. For the Quasi-Periodic type 2 microstructure, no widening of the wave-packet occurs

starting $\lambda_{in}/d = 8$, for wavelengths $\lambda_{in}/d \leq 7$, dominance of the diffusive transportation regime is observed.

Combining the different proposed criteria draws the line on the transition from the diffusive to the propagative regime.

To shed more light on the amplitudes and wavelengths at stake in the microstructures' as the wave-packet travels within, the velocity at the output V_{out} is analysed in the frequency domain for the whole range of λ_{in} .

4.7 Frequency components at outlet

In this section, a study on the wavelengths components of the output velocity V_{out} is carried-out. The goal is to reveal the role played by the microstructural hole distribution, not only on the attenuation of the stress-waves as seen previously, but also on the individual wavelengths contributing to the velocity of the material points at the outlet. The choice of considering the velocity instead of the kinetic energy is to ensure a more straightforward physical interpretation of the results.

Figure 4.12 shows the evolution of the material velocity as the stress-wave packet reaches the right side of the sample (the outlet, after it travelled through the microstructure). Since the considered geometry consists of the microstructure embedded inside a rectangular sample (Figure 4.9), the outlet velocity can be analysed in space, i.e., the evolution in time of the velocity at the outlet can be transferred to an evolution in space via the known wave-speed of the bulk material; this allows an analysis of the wavelengths recomposing the outlet velocity.

It's noted that for each i -wavelength, the plots are normalised by their corresponding maximum for a better visualisation. The lower row of images (Figure 4.12) shows typical *FFT* analysis results on the outlet velocity reported in terms of the characteristic wavelength d of the materials. Three wavelengths of interest are shown for each microstructure. For the Periodic microstructure (Figure 4.12(a)), $\lambda_{in}/d = 4, 7$ and 9 are shown. *FFT* analysis on V_{out} of the smallest wavelength shows two dominant peaks at two wavelengths $\lambda_{out}/d = 3, 4.66$ on each side of the input wavelength $\lambda_{in}/d = 4$. Similar response is obtained at $\lambda_{in}/d = 7$. At $\lambda_{in}/d = 9$, it's clear that the same frequency as the excitation is recovered at the output.

For the Quasi-Periodic type 1 microstructure (Figure 4.12(b)), $\lambda_{in}/d = 4, 6$ and 9 are considered. *FFT* analysis on V_{out} of the smallest wavelength shows the same frequency

at the output as the excitation frequency. At $\lambda_{in}/d = 6$, the dominant wavelength at the outlet of the microstructure is shifted to $\lambda_{out}/d = 7$. At $\lambda_{in}/d = 9$, the same frequency is recovered at the outlet. It's recalled that the influence of the attenuation is **not** taken into consideration in this analysis since the amplitudes are normalised by their maximum value.

For the Quasi-Periodic type 2 microstructure (Figure 4.12(c)), $\lambda_{in}/d = 4, 6$ and 9 are considered. Contrary to the type 1 microstructure, the smallest wavelength $\lambda_{in}/d = 4$ is not recovered and the dominant peak at the outlet is shifted to $\lambda_{out}/d = 5$. The dominant frequency at $\lambda_{in}/d = 6$ is recovered, and another peak emerges at $\lambda_{out}/d = 6.66$. At $\lambda_{in}/d = 9$, it's clear that the same frequency as the excitation is recovered at the output.

By analysing input wavelengths ranging from $\lambda_{in} = d$ to $\lambda_{in} = 10d$, the *FFT* results can be juxtaposed in a $(\lambda_{in} - \lambda_{out})$ space, along with the contribution of each output frequency into V_{out} creating thus an extensive input-output frequency map (IOFM) relative to each microstructure.

The IOFM of the Periodic, Quasi-Periodic type 1 and 2 microstructures are shown in Figure 4.13. The excitation wavelengths studied previously (Figure 4.12) are represented by the yellow dashed-lines; plus, the identity ($y = x$) function in the $(\lambda_{in} - \lambda_{out})$ space is represented by the dashed green lines.

The IOFM of the Periodic microstructure (Figure 4.13(a)) shows a **large complete band-gap** around $\lambda/d = 3.5 - 4.5$, a result coherent with [Saleh, 2017]. For smaller wavelengths $\lambda/d = 1 - 3$, although the previously shown scattering of the wave-packet, the frequency at the outlet is similar to the excitation frequency. We recall that the attenuation is dismissed by means of the normalisation. For input wavelengths $\lambda/d = 2.5 - 4$, the dominant output wavelengths are centred at $\lambda_{out}/d = 3$, it's mentioned that the input wavelength $\lambda_{in}/d = 3$ had a special behaviour inside the Periodic microstructure. For $\lambda/d = 2.5 - 3$, a complete band-gap appears. **Partial band-gaps** are also present at different wavelengths, with the largest partial bandgap shown at $\lambda_{out}/d = 2.5 - 3$. At partial band-gaps, the corresponding frequencies are not blocked entirely and only a small amount of the energy is transported. As shown, in the IOFM, with increasing the excitation wavelength, the output frequencies are separated by partial bandgaps (e.g., $\lambda_{out}/d = 5, 5.5, 7, 7.66 - 8.66, 9.66$, etc.) and are centred at specific wavelengths (e.g., $\lambda_{out}/d = 4.66, 6, 7.5, 9, 10.5$, etc.).

The IOFM of the Quasi-Periodic type 1 microstructure (Figure 4.13(b)) shows two large complete band-gaps between $\lambda/d = 1$ up to $\lambda/d = 4$ and then from $\lambda_{out}/d = 4$ to $\lambda/d = 6$. It's noted that the specific wavelength λ_{out}/d is the common dominant wavelength for

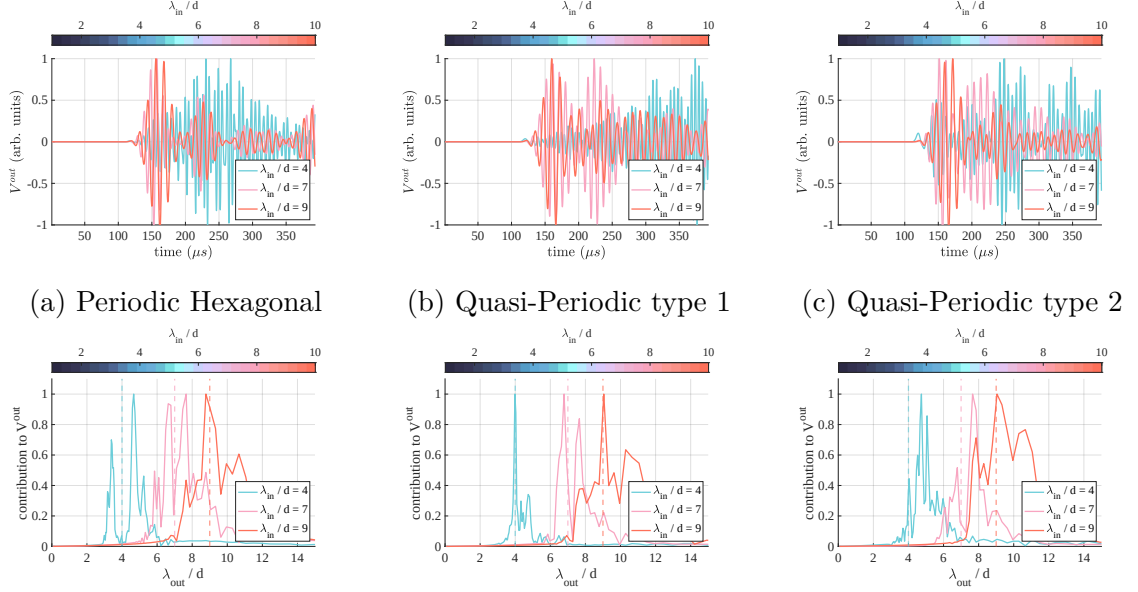
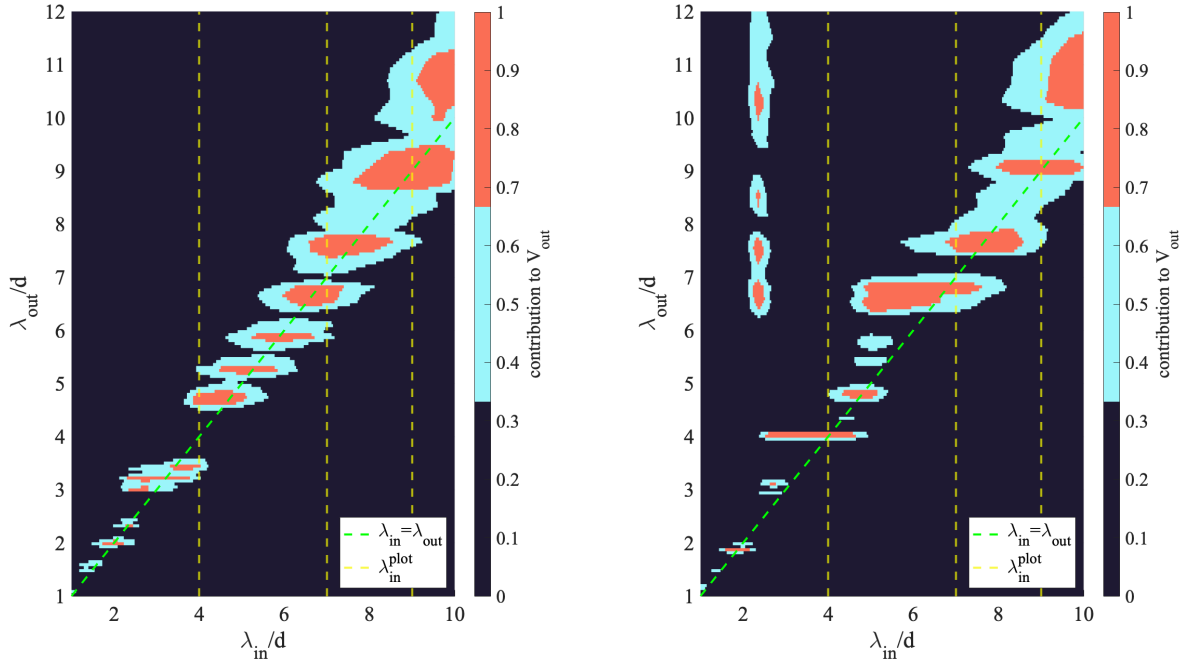


Figure 4.12 – Velocity evolution in time at the outlet V_{out} and its FFT analysis for the Periodic (a), Quasi-Periodic type 1 (b) and Quasi-Periodic type 2 (c). The velocities V_{out} are normalised for visualisation purposes. The FFT results show the contribution of different wavelengths to V_{out} .

excitation wavelengths going from $\lambda_{in}/d = 2.5$ to $\lambda_{in}/d = 5$. A similar unique dominant wavelength appears at $\lambda_{out}/d = 6.5$. A thinner bandgap appears around $\lambda/d = 7$. A partial band-gap appears around $\lambda/d = 9 - 10$.

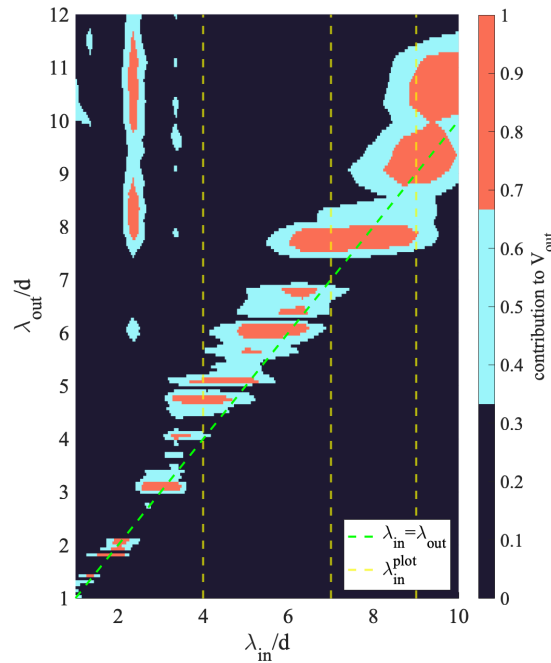
The IOFM of the Quasi-Periodic type 2 microstructure (Figure 4.13(c)) shows two large complete band-gaps between $\lambda/d = 2$ and 3. A thinner bandgap appears around $\lambda/d = 7$. A partial band-gap appears around $\lambda/d = 7 - 7.5$. A partial band-gap appears around $\lambda/d = 5.5 - 6$. Unique dominant wavelength appears at $\lambda_{out}/d = 5$ and $\lambda/d = 7.8$ for excitation wavelengths going from $\lambda_{in}/d = 3$ to $\lambda_{in}/d = 5$ and $\lambda_{in}/d = 6$ to $\lambda_{in}/d = 9$ respectively.

As seen, more light is shed on the amplitudes and wavelengths at stake in the microstructure as wave-packets travel through. The presence of different band-gaps for each microstructure is observed, as well as the presence of partial bandgaps in all three microstructures. If the output frequencies in the Periodic microstructure are aligned along the identity function with broadening as the excitation wavelength increases, the response of the Quasi-Periodic microstructures shows a horizontal shift that can be explained by the larger amount of scattering and thus high frequency (low wavelength) in the output velocity.



(a) Periodic Hexagonal

(b) Quasi-Periodic type 1



(c) Quasi-Periodic type 2

Figure 4.13 – Input-output frequency map (IOFM) of the Periodic, Quasi-Periodic type 1 and type 2 architected materials.

4.8 Concluding remarks

The attenuation of the stress-waves inside the Periodic and Quasi-Periodic architectures is put-forth in this chapter. 2D FE simulations follow the evolution of wave-packets of different wavelengths through the samples. The kinetic energy attenuation performance is compared between the Periodic hexagonal architecture and the two kite&dart Quasi-Periodic architectures. The amazing capabilities of the Quasi-Periodic microstructure to damp the stress-waves is noted; in fact, unlike in the hexagonal architecture (where only one length characterises the structure (d)), the long-range pattern heterogeneities in the Quasi-Periodic microstructures provide continuous source of scattering leading to an increase in the diffusivity and attenuation accompanied with a decrease in the penetration length.

Besides, separate regimes of energy transport are found and well established; those transport regimes evolve as the excitation wavelength changes. The identification of the transport regimes has been possible by relating the energy at the outlet to the spreading of the initial excitation into **coherent** and **incoherent** vibrations: the propagative part being the coherent contribution to the transfer, and the diffusive one being the incoherent part.

Moreover, we show how the instantaneous wave-speed is reduced at small wavelengths, due to the scattering and the redistribution of the kinetic energy in directions different than the principal direction of propagation. No plateau is reached in neither Quasi-Periodic microstructures (in the studied range of wavelengths of course).

Note that the system is purely harmonic here (except for the silent boundary conditions SBC), which means that the dissipation of energy between the inlet and the outlet is only an effective dissipation of energy resulting from waves spreading due to scattering inside the architecture between the inlet and outlet. The imposed SBC being away from the analysed zone do not contribute to the studied part of the energy dissipation, and are only considered to mimic an infinite medium reducing boundary effects and preventing unwanted reflection. So one can see the architecture as a filter embedded in an infinite medium and modifying the stress-wave packet as it wishes.

Further, this chapter shed light on the wavelengths components of the wave-packet exiting the considered microstructures. Bandgaps are shown to exist in the three microstructures, with an increase in the Quasi-Periodic microstructures, a signature of their long-range heterogeneities in their patterns. Herein shown results join recent findings by

[Glacet, 2019] that show the possible existence of band-gaps in the vibrational response of Periodic and Quasi-Periodic beam lattices.

The superiority of the Quasi-Periodic microstructures is once again advanced as we relate their overall better dynamic properties (stress-wave scattering, attenuation, bandgaps, etc.) compared to the Periodic microstructure.

It's believed that these results are of high relevance as they allow the microscopic understanding of the influence of the architecture's periodicity on the transport of mechanical energy. More importantly, in the context of this thesis, regarding the analysis of fracture in architected materials, this chapter elaborates on the stress-waves' behaviour a crack would encounter if it were to advance dynamically within such materials.

The next and final chapter, is devoted to the study of the influence of stress-waves on crack propagation.

Open issues and extensions

- In this study, a single r_h/d ratio is studied which means that the comparison was restrained to the influence of the periodicity of the microstructure on the damping properties and vibrational properties.
- The consideration of a finite element method to analyse the dynamic properties of the Periodic and Quasi-Periodic architectures required huge computational resources. Of course analytical solutions exist for the Periodic architecture, and numerical methods based on the construction of boundary value problems on *RVE* exist. However, since an *RVE* cannot be accurately defined in the case of non-periodic microstructures, and to overcome any probable bias coming from the consideration of approximate *RVEs*, we restricted the study to $d \leq \lambda_{in} \leq 10d$.
- As mentioned in the chapter, periodic boundary conditions can be considered for the analysis [Luo et al., 2021, Glacet, 2019], for the Periodic microstructure on an *RVE*, and for periodic approximation of the Quasi-Periodic ones. However, as the approximation might induce some unwanted bias, the decision to consider the same numerical model for the different microstructures was carried-out.

STRESS-WAVES AND THEIR ROLE IN CRACK PROPAGATION

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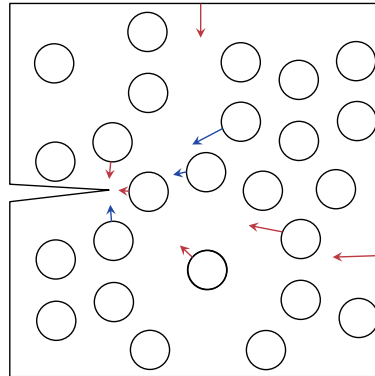


Figure 5.1 – crack-tip in architected materials: a schematic representation stress-waves reflections from the free boundaries of the architecture

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5.1 Introduction

In Chapter 3, the quasi-static propagation of a crack inside the architected materials is studied. At the microstructural level, it shows the attraction of the crack-tip to the holes, it shows also the presence of a preferential weak plane for propagation in the Periodic microstructure, and the presence of 'resilient zones' in the Quasi-Periodic material. In the previous Chapter 4, the stress-wave interaction with the architectures' microstructure is studied. Attenuation of the stress-waves resulting from wave spreading due to the continuous scattering at the free boundaries of the architecture is put forth.

Imagine a crack-tip immersed in such architectures (Figure 5.1). Under dynamic loading (rapidly varying loads, high strain rates, etc.), the crack-tip would 'see' continuous variation of the stress states in its vicinity coming from the back-and-forth reflections of the stress-waves at the free boundaries of the architecture. To be able to understand the dynamic crack propagation in such materials, the influence of stress-waves on the stress-state at the crack-tip and eventually on the crack growth must be carefully characterised.

Even in homogenous materials, the problem is complex since stress-waves load the crack-tip. Therefore the stress-field at the crack-tip is continuously changing as the stress-waves travel inside the material. And depending on the boundary conditions, the crack can alternatively, be loaded and unloaded.

We believe that understanding the interaction between stress-waves and crack-tip(s), debuting with homogenous materials, should build the foundation for future analysis of the dynamic fracture of architected materials, i.e., where a range of mixed and complex stress-waves reflections and interactions with the crack-tip and the microstructures are expected.

5.1.1 ...and more

If in statics, fracture mechanics relies on the balance between fracture energy and the strain energy release rate, the game in dynamics is much more complex and this inherent difficulty arises from the strong interactions between the crack-tip stresses, crack-tip speeds, but also with the stress-waves reflected from the boundaries and those emitted by the crack-tip itself. Dynamics fracture mechanics thus relies on the balance between the fracture energy from one side and the dynamic energy release rate from the other; the latter being affected by the redistribution of the stresses at the crack-tip [Bleyer et al., 2017]. Dynamic fracture mechanics also predicts that the Rayleigh wave speed c_R is the limiting velocity of a mode I stable crack propagation. However, experimental observations show the existence of limiting velocities typically around 40% of c_R , above which instabilities emerge and eventual branching occurs¹. Besides, phase-field approaches to dynamic fracture are shown to successfully reproduce experimental crack patterns, i.e., initiation, coalescence, branching positions and branching angles. In the same spirit as in the experiments, it is found that the tip speed of stable cracks in phase-field simulations are also limited around the same order of magnitudes ($\sim 40\%$ of c_R) as the experiments (with some discrepancy). However, accurate experimental setups to validate the phase-field predictions regarding the crack history and tip speeds are usually insufficient, and the predictions are usually validated *post-mortem* on the crack patterns only.

The instantaneous crack (in)stabilities, i.e., branching, turning and limiting velocities under mode I are at the core of this chapter; more specifically, the ability to explain crack branching at slower tip speeds than the ones predicted via the dynamic fracture mechanics is sought.

Unlike in previous chapters, where the numerical simulations of damage are at the core of the developments, this chapter is based on dynamic fracture mechanics concepts applied on a novel experimental setup. Interesting phenomena regarding the crack propagation's

1. The limiting velocity is found to depend on the material, the geometry and boundary conditions.

interaction with stress-waves are expected. The amazing technologies at Ecole Centrale de Nantes: an Ultra-High-Speed-High-Resolution UHS-HR camera and digital image correlation *DIC* skills, offer insights on the extraordinary phenomena governing crack propagation and crack (in)stabilities, and enable the definition of what we call 'material (in)stability map', a comprehensive criterion for crack branching.

This chapter is organised as follows: the novel experimental setup is briefly introduced. The *DIC* displacement fields, the derived crack-tip speeds and *post – mortem* crack patterns are then presented. Here, questions related to the crack path history and branching conditions are asked: **when** and **why** does the crack branch? If the first answer can be easily answered by following the opening of the crack directly from the images, the second question is a bit more tricky.

As mentioned, the answer is sought following the basic dynamic fracture mechanics concepts; therefore the influence of the crack-tip speeds on the angular stress distribution from [Yoffe, 1951] is first recalled, and the inability to explain branching at low crack-tip speeds is stressed. The analysis of the angular stress distribution as a criterion for crack (in)stability is retained, however, we build on the work of [Ramulu and Kobayashi, 1983] and introduce higher order terms in the analysis.

To elaborate on the experimental instabilities, quantities relevant to fracture mechanics knowingly *SIF*, higher order terms and crack-tip positions in time are extracted from the displacement fields via the method proposed by [Roux and Hild, 2006, Roux et al., 2009]. The angular stress distribution is investigated from the elastodynamics solution of the stress field. At branching, this shows indeed a deviation of the maximum circumferential stress from its principal direction along the crack extension, which can clearly account for the branching.

From here, we build a material (in)stability map that embodies a criterion for the transition between stable and unstable crack propagation. The criterion is valid under all crack-tip speeds $0 \leq v_c \leq c_R$, with the unquestionable role of *T – stress* (higher order term) on crack instability at its core.

A methodology to experimentally (and numerically) advocate the instability source at the bifurcation position is hence proposed. To wrap-up this chapter, we get back to [Borden et al., 2012]'s benchmark in which -unlike the proposed experiment- no external loading along the direction of crack propagation is considered, yet branching occurs. Unsurprisingly, the methodology successfully predicts the (in)stability conditions and the branching angle, but also gives insights on the damage band thickening in phase-field.

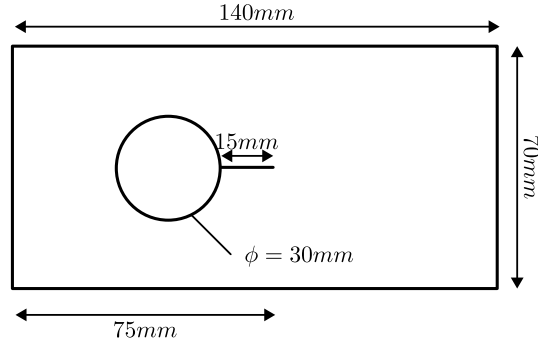


Figure 5.2 – Sample geometry and dimensions for the inertial impact test [Grégoire et al., 2007]. The hole converts the compressive wave from the input to a tensile loading at the notch

5.2 Crack branching in an inertial impact test

This first section briefly describes the experimental and imaging setup of the inertial impact test. The experiments were performed at **CRED : Centre de Ressources en Essais Dynamiques**, in Ecole Centrale de Nantes.

The specimen geometry from [Grégoire et al., 2007] is combined with the test configuration from [Pierron et al., 2014] to enable interesting crack propagation interaction with stress-waves; knowingly:

- compressive waves from the impact are converted to tensile ones and initiate the crack propagation;
- the propagating crack meets reflected stress-waves from the boundaries and bifurcates into two symmetric branches.
- the two branches propagate at similar velocities.

All these phenomena and more will be investigated in details.

5.2.1 On the shoulders of giants

[Grégoire et al., 2007] analysed a Split Hopkinson Pressure Bar (SHPB) test (low impact velocity $\sim 10m/s$) via numerical simulations. For this, he used a distinctive geometry that

enabled compelling crack propagation behaviour: a rectangular plate ($140\text{mm} \times 70\text{mm}$) with a hole of diameter $d_h = 30\text{mm}$. The circular hole is vertically centred at a distance $d_h = 45\text{mm}$ from the border. A 15mm notch is cut out as in (Figure 5.2). The impact should induce compressive waves; however, the presence of the hole creates a tensile zone sideways of the hole opening thus the notch and enabling the fracture. Different propagation phases were observed in his work showing compelling interactions between stress-wave and the crack: (i) the crack is initiated and propagates at a constant velocity, (ii) it stops (arrested), (iii) and then restarts at a constant velocity (slower than in the first phase).

Conversely, [Pierron et al., 2014] went 'beyond Hopkinson's bar' and provided a seminal test configuration called the inertial impact test. In this type of tests, the specimen is impacted and 'left on its own'; indeed, the specimen is loaded by a short pulse (due to compressive waves from the impact). By exploiting advancements in full-field measurements, identification of material properties is possible from camera recordings and full-field measurements without the need for external forces².

The available cutting edge technologies (gas gun, UHS-HR camera) combined with advanced *DIC* skills³ (in-lab-developed state-of-the-art calibration methodology [Vinell et al., 2021]), at Ecole Centrale de Nantes, enabled the investigation on advanced experimental configurations inspired from [Pierron et al., 2014] and [Grégoire et al., 2007]: where full-field measurements of a high-velocity impact ($\sim 30\text{m/s}$) are exploited to extract meaningful fracture mechanics quantities (*SIF*, *T* – stress, crack-tip position, crack-tip speeds, etc.) and to analyse the fracture behaviour.

5.2.2 Loading and test configuration

The specimen shown in Figure 5.2 is to be loaded dynamically via an impact on the edge perpendicular to the notch as schematised in Figure 5.3. The impact should induce a compressive wave; however, the presence of the hole creates a tensile zone sideways opening thus the notch and enabling the fracture [Grégoire et al., 2007]. As compared to [Grégoire et al., 2007], the absence of an impedance at the right-hand side boundary (in his case, the use of Hopkinson's bars with similar mechanical properties to those of the

2. As advanced, [Pierron et al., 2014], inertial effects are usually a burden for the measurement of external forces, altering the identification of the material behaviour

3. The open-source in-lab-developed software UFreckles is provided via <https://zenodo.org/record/1433776>



Figure 5.3 – A schematic representation of the experimental configuration

specimen), stress-waves will be reflected from the right-hand side boundary and will deliver new loading-unloading conditions of the crack-tip probably modifying its advancement (as we'll see shortly). The specimen is mounted on a waveguide to ensure proper compressive wave entering the specimen [Van Blitterswyk et al., 2018, Vinel et al., 2021], and to hold the sample while keeping all other boundaries free.

Remark 5.1. *To give the reader more insights on the global phenomena happening after the impact, the **Lagrange representation** of the impact (projectile-waveguide-specimen) is detailed in Appendix E. And of course, the main focus will consequently be drawn on the last part of the impact, i.e., the loading of the specimen.*

5.2.3 Experimental and imaging setup

The sample is laser-cut from a commercial PolyMethyl Methacrylate (PMMA) manufactured by Arkema; to apply the *DIC*, a synthetic speckle pattern is laser-engraved into the sample following [Vinel et al., 2021].

The projectile and the waveguide are machined from a polyoxymethylene (POM) cylinder of diameter $d_{proj} = d_{wg} = 40mm$; both are $80mm$ long. POM is used because it has similar material properties as PMMA (More on the identification of the elastic properties of PMMA in Subsection 5.2.7). The projectile is fired by a gas gun to reach a velocity of V_{proj} just before the impact (impact with the waveguide on which the specimen is mounted). A shock absorber is needed to neutralize the impact.

All images are captured using the UHS-HR Cordin Model 580 (at $400k$ fps with a resolution of $3296 \times 2472px$). To provide enough lighting for the camera sensors, additional lighting is provided by two Pro-10 Profoto flashes ($2 \times 2400J$ provided in $1000\mu s$). The flashes are triggered via an infrared light-gate system (SPX1189 series Honeywell) mounted

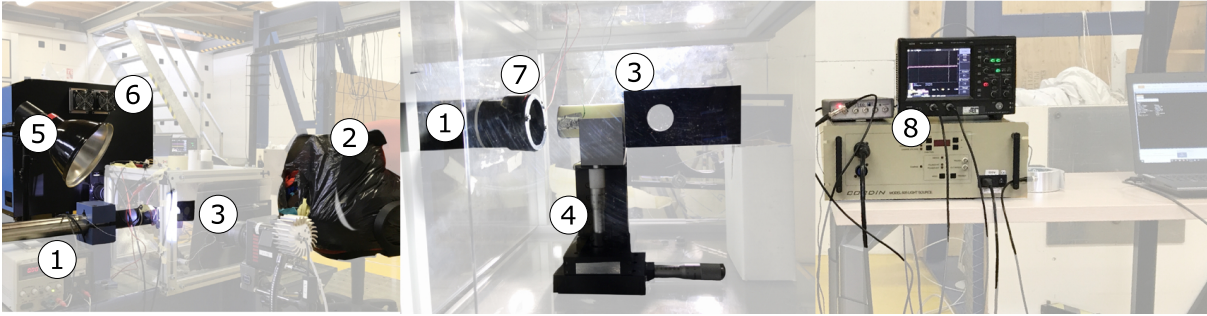


Figure 5.4 – Experimental set-up for the inertial impact tests

at the end of the gas gun.

At such $400k$ *fps* and $3296 \times 2472px$ resolution, the camera records the entire test: from the first compressive waves induced by the impact to the total failure of the specimen (about $200\mu s$, 78 frames). A photo of the test bench can be found in Figure 5.4. One identifies:

1. The gas gun
2. The shock absorber
3. The specimen mounted on the waveguide
4. The PMMA support bed on the optical positioners
5. The flash lights
6. The UHS-HR camera: the Cordin Model 580
7. A light-gate: the SPX1189 series Honeywell infrared sensor
8. The delay generator (to synchronise the flashes, more details in Appendices F.1)

Details about the **experimental and imaging setup** can be found in the Appendices F.1 to avoid overloading the chapter.

A series of impact tests (Figure 5.3) were performed at Ecole Centrale de Nantes. Four representative samples are analysed (designated TAF1, TAF2, T3DE and THOM). In this chapter, only results and full-field measurements of the TAF1 sample will be detailed. Related material to TAF2, T3DE and THOM are showcased in Appendices G, H I, respectively.

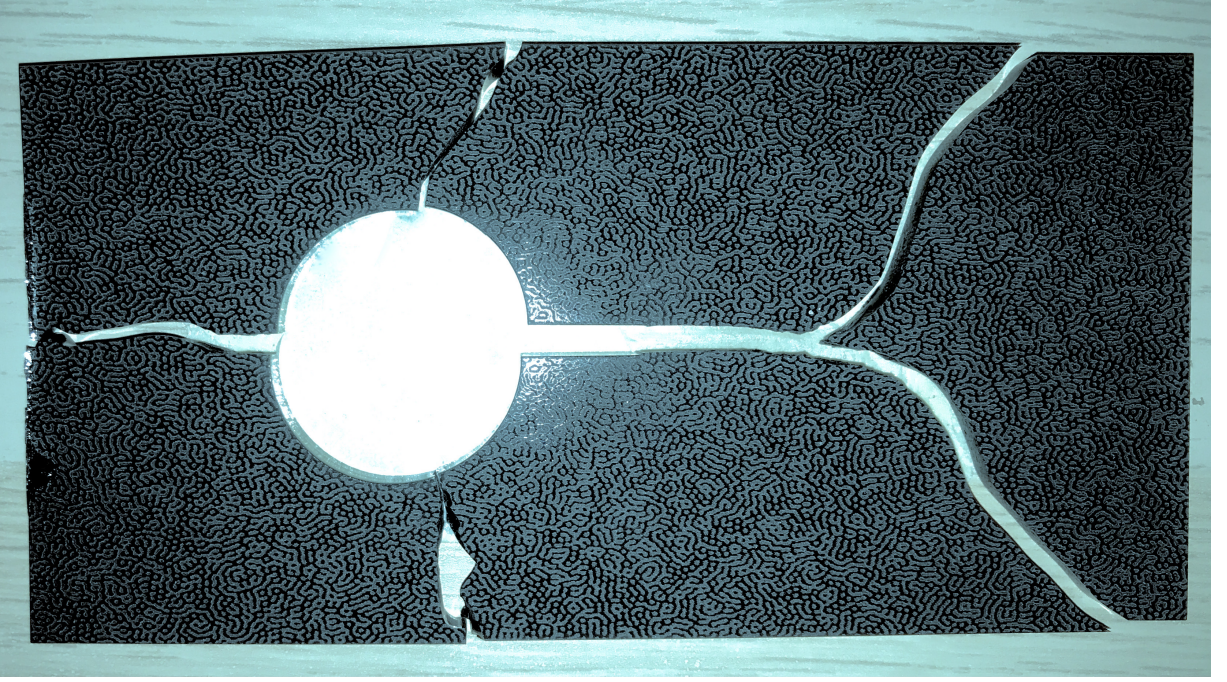


Figure 5.5 – *Post-mortem* photograph of sample TAF1 (impact velocity $V_{proj} = 30.5m/s$)

5.2.4 *Post-mortem* state of the sample

By precautionarily setting the gas guns pressure to $1.49atm$ and $1.55atm$, the projectile's speed⁴ just before the impact was respectively around $20m/s$ and $30m/s$ ($22m/s$ for TAF2 and THOM, $30.5m/s$ for TAF1, and $31.8m/s$ for T3DE).

Figure 5.5 shows the crack(s) paths on the sample TAF1 (*post-mortem*). As seen, a first crack is observed at the left-hand side of the hole. Undoubtedly, Poisson effect coming from the horizontal compression is responsible for the initiation. A little curve on the crack suggests a small misalignment in the mounting of the specimen on the waveguide. On the right, a crack is initiated from the notch, it travels horizontally ($24mm$) before branching into two branches (at an angle $\theta = +40^\circ$ and $\theta = -15^\circ$). Each branch displays two convexities; stress-wave reflection at the free boundaries are expected to play a predominant role on these deviations. Two vertical cracks are also present at each side of the hole.

The samples consistently show the same crack patterns (Appendix G for TAF2 and H for T3DE) suggesting a repeatability of the setup, and interesting phenomena waiting to

4. The projectile's speed is computed from images taken at lower frame rate, ($10000fps$) with a standard high speed camera

be explored.

Highly resolved ultrafast imaging combined with *DIC* enables the validation of the big role played by the stress-waves on the cracks patterns.

Before exploring the measurements, we give some remarks regarding the *DIC* data processing.

Remark 5.2. *Unlike in statics where standard cameras are used and where DIC yields accurate measurements, in dynamics, especially when recording with an UHS-HR rotating camera at 400kfps, neat imaging cannot be achieved. Despite the application of the novel calibration method from [Vinel et al., 2021] to suppress apparatus induced distortions, residual distortions may remain introducing a bias in the DIC measurements.*

Remark 5.3. *The displacement fields are filtered in time with a Savitzky Golay (kernel size= 5 frames, order 2) filter to smoothen the first derivative (velocity fields); moreover, spatial noise is filtered out via a Tikhonov regularisation of the DIC problem.*

Remark 5.4. *The strain-rate fields are derived by spatial differentiation of the velocities; velocities are derived from temporal differentiation of the displacement fields.*

Remark 5.5. *The time origin ($t = 0$) corresponds to the camera trigger.*

Remark 5.6. *The initiation and the bifurcation frames are determined from the opening of the crack lips (twin nodes along the crack path) in the images from the UHS-HR camera.*

Remark 5.7. *The opening of the crack lips along the crack path (twin nodes along the crack path) allows the computation of an apparent crack-tip speed.*

Remark 5.8. *The apparent speed computed from the opening of the twin nodes along the crack path is only a rough estimation of the actual crack-tip speed since it can be affected by local noise, lighting of the crack lips and pixel resolution. A more precise estimation will be determined following [Roux and Hild, 2006, Roux et al., 2009] in the next section. His method is based on the analysis of the elastic fields in the sample, determining thus more accurately the crack-tip position (sub-pixel precision) and derivating its speed. The methodology for the estimation is given in Appendix D.*

5.2.5 *DIC* displacement fields

Figure 5.6 shows displacement fields, longitudinal and transverse strain rate fields of the TAF1 specimen at three different time steps. The following phenomena occur around

these time steps: at $10\mu s$ (figures on the left), the first stress-waves entering the specimen are shown, at $60\mu s$ (figures in the middle), the crack on the right-hand side of the hole is initiated from the notch, at $95\mu s$ (figures on the right), the crack bifurcates into two branches.

For the other specimens, see Appendices [G](#), [H](#), [I](#)

The ability to register 78 snapshot at $400kfps$ enables capturing never-seen-before details regarding stress-wave and crack propagation. The apparent crack-tip speeds are shown in Figure [5.7](#). The most compelling phenomena are listed under ►.

- The initiation of the impact and the first compressive waves enter the specimen (at $500s^{-1}strain - rates$, shown at $t = 10\mu s$ in Figure [5.6\(d\)](#));
- The role of the hole in creating traction zones sideways (at $t = 10\mu s$ in Figure [5.6\(g\)](#)),

As seen in the previous section [5.2.4](#), two main cracks are observed sideways of the hole (a first one at left-hand side of the hole and another one from the notch). Observation from the *DIC* displacement fields show that surprisingly,

- the crack at the left-hand side of the hole is first initiated ($t = 40\mu s$). Once its length reaches $15mm$,
- the second crack initiates from the notch at the right-hand side of the hole (at around $t = 60\mu s$).

After initiating from the notch around ($t = 60\mu s$), the crack accelerates to around velocity of roughly $700m/s$ corresponding to $0.55c_R$.

- Compressive stress-waves are reflected as traction waves from the right-hand side boundary, and they overlap the tip of the crack.

The crack decelerates and reaches the branching position while travelling at around $v_c = 650m/s = 0.5c_R$.

- Bifurcation of the crack into two branches happen at $t = 95\mu s$.
- The two branches advance at particularly close velocities.
- Complex stress-wave orthogonal to the crack branches supposedly deviate the branches.

Even though the same geometry as [[Grégoire et al., 2007](#)] is used, it's clear that the stress-wave propagation history is fundamentally different (the absence of an impedance

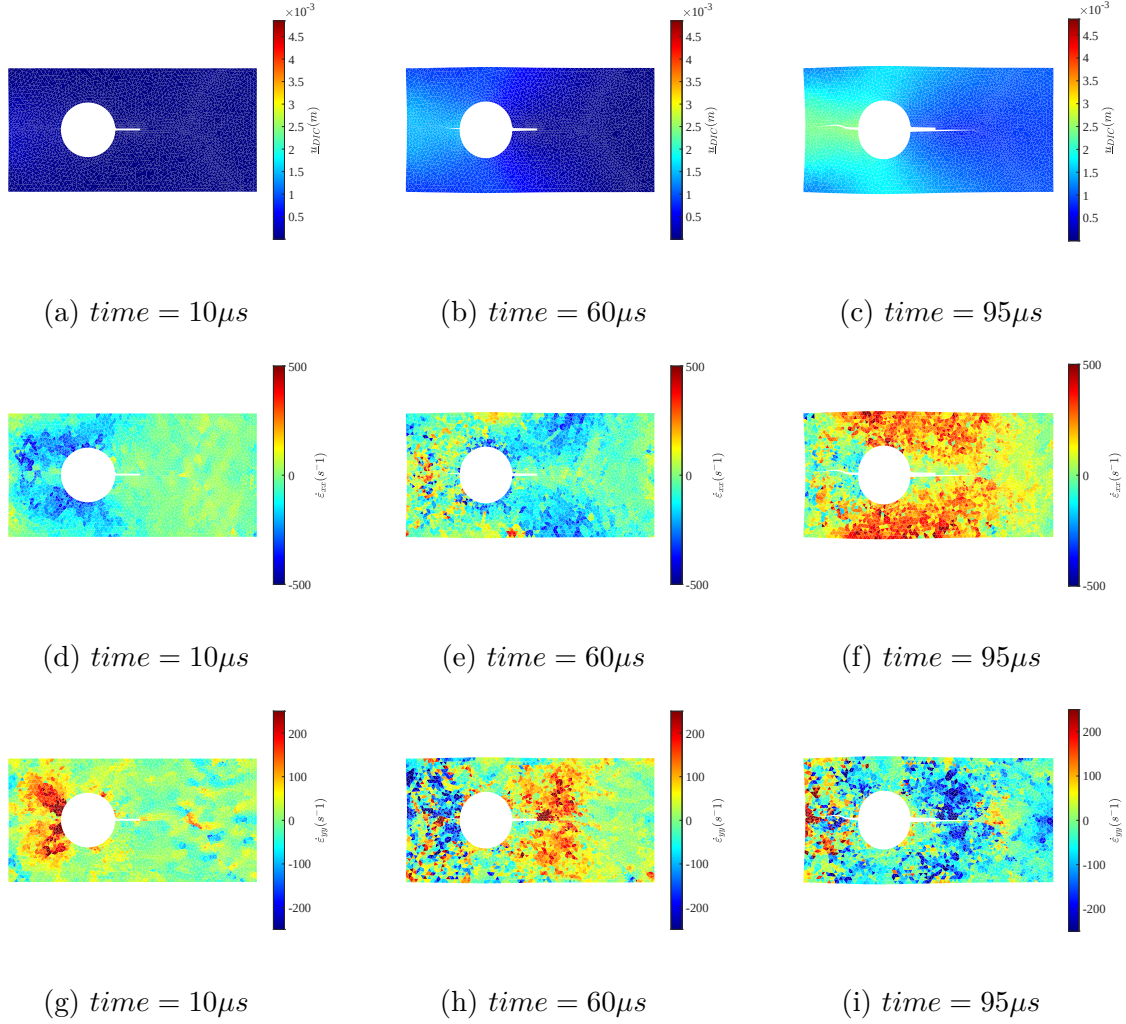


Figure 5.6 – Sample TAF1 - *DIC* displacement fields (up), longitudinal (middle) and transversal (down) strain rates at three time steps. A Savitzky Golay (kernel size= 5 frames, order 2) filter smoothens the displacements' first derivative (velocity fields). Spatial noise is filtered-out via a Tikhonov regularisation of the *DIC* problem

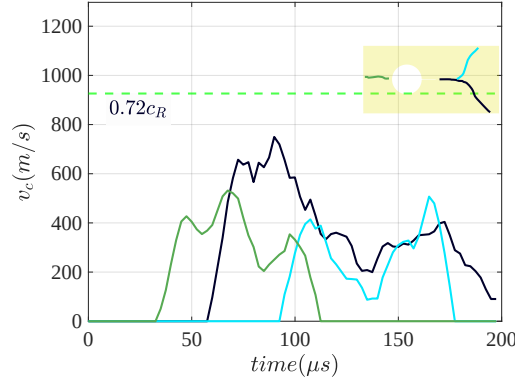


Figure 5.7 – Experimental apparent crack-tip speeds of TAF1 sample obtained from the crack opening

at the right-hand side of the specimen). Stress-wave reflections from the right-hand side boundary deliver new loading-unloading events of the crack-tip, which indeed enables distinctive crack patterns.

5.2.6 On the crack branching

The ability to quantify the rich dynamical behaviour of the cracks (initiation, acceleration, deceleration, branching) was enabled thanks to the novel experimental setup and the advanced *DIC* skills.

The focus is shed on the branching phenomenon. As observed, the branching occurs after a certain duration of time in which the main crack appears to be decelerating. Questions regarding the presence of a **limiting velocity** from one side and regarding the crack **branching at lower crack-tip speeds** from the other are asked.

As mentioned, the answers are sought using a simple dynamic fracture mechanics concept: the **angular distribution of the stresses**.

It is assumed that fracture is driven by the stress, and that the crack will propagate in the direction of maximum circumferential stress [Erdogan and Sih, 1963, Streit and Finnie, 1980, Finnie and Saith, 1973]. The aim is to successfully predict the crack propagation direction only via **fracture-mechanics-related quantities**.

For this purpose, we estimate the *SIF*, *T – stress*, the crack-tip position and derivate the crack-tip speed v_c from the experimental full-field kinematics following [Roux and

Hild, 2006, Roux et al., 2009]⁵. This enables the assessment of the angular distribution of the stresses along the crack propagation (between the notch and the branching position) through the following steps:

$$\underline{u}_{DIC} \rightarrow SIF, T - stress, \text{ crack-tip position, and } v_c \rightarrow \sigma$$

where $\underline{u}_{DIC}$ is the *DIC* displacement field from which fracture mechanics relevant quantities can be extracted. *SIF*, *T – stress*, crack-tip position, and v_c are then injected in the analytical solution of the asymptotic fields [Freund and Hutchinson, 1992] to compute σ .

We'll see how adding the higher-order term *T – stress* in the stress solution is reflected on the **modification of the direction of crack propagation** at the **branching position** (where the crack advances at v_c lower than the threshold predicted by the classical solution) which eventually translates to branching (crack instability). From there, we generalise this finding by constructing an **(in)stability map** that embodies a criterion for crack instability.

In the next section, we commence by showcasing the *SIF*, *T – stress* and crack-tip speed results computed directly from the *DIC* displacement fields, as intermediate results from the analysis scheme.

5.2.7 *SIF*, *T – stress* and crack-tip speed

Having full-field measurement of the kinematics of a specimen, one can estimate the crack-tip position (and crack-tip velocity), the *SIF* and higher order terms (e.g., *T – stress*) from Williams' expansion automatically following [Roux and Hild, 2006, Roux et al., 2009]. In brief, by projecting displacement fields in a zone around the crack-tip on the analytical solution proposed by [Williams, 1957], relevant quantities can be estimated. We recall that the methodology, its parameters and its application scheme are described in Appendix D;

The elastic properties of the material are required to be known to estimate these quantities. The elasticity tensor is determined via an **in-house FEMU** (Finite Element Model Updating Method) identification method. Table 5.1 summarises the identified material properties under the plain strain assumption. Interested readers are referred to Subsection 5.2.7 for a brief note on the PMMA properties.

5. The methodology is briefly introduced in Section 5.2.7, and detailed in the Appendix D for interested readers

ρ	$1200kg/m^3$	c_d	$2594m/s$
E	$6GPa$	c_s	$1387m/s$
ν	0.3	c_R	$1287m/s$

Table 5.1 – Material properties for the PMMA identified from the full-field measurements via the in-house FEMU identification method

Discussion on the behaviour of PMMA

Even though PMMA exhibits viscoelastic material properties, it is hard to identify the effective viscoelastic parameters due to the complexity of loading and unloading (inertial effects). From here, it is assumed that the samples exhibit linear elastic behaviour, with a modification on the elastic properties to take the viscoelastic effects into account. An in-house FEMU is considered. The advantage of this method as implemented over other methods (the virtual fields method [Grédiac, 1989] for example) is that it allows the direct identification of the full elasticity tensor $\mathbb{C}$ of the material with **no *a priori*** on the plane strain plane stress assumptions, and is also applicable for coarse temporal discretisation. The effective elasticity tensor is then identified from full-field measurements from the time of impact until the time steps preceding the initiation of the first crack. The identified material properties are summarised in Table 5.1. This identification procedure is repeated for the different samples TAF1, TAF2, T3DE, THOM and similar properties are determined.

SIF , T – stress and crack-tip speed

Figure 5.8 shows the extraction results, namely SIF , T – stress and the crack-tip speed v_c . The robustness of the extraction (vis-à-vis its parameter, i.e. sizes of extraction zones, Appendix D) is also reported by the error-bars .

The relatively wide error-bar of crack-tip velocity (purple) at the initiation (around $t = 60\mu s$) suggests a high sensibility of the estimation to the extraction zone size. After $t \simeq 95\mu s$, the different error-bars also broaden. These widenings can be explained by the following: before $t = 60\mu s$ there are no cracks in the region of interest (right-hand side of the hole); after $t \simeq 95\mu s$, crack branching occurs.

Remark 5.9. *The extraction (SIF , T – stress, v_c) holds solely between the moment of crack initiation (around $t = 60\mu s$) and the moment of branching around $95\mu s$. Afterwards, a redistribution of the stress states occurs due to the coexistence of two neighbouring*

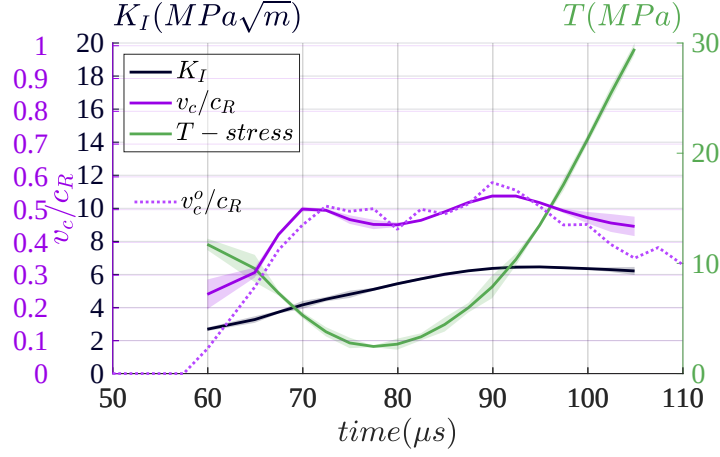


Figure 5.8 – Experimental SIF , the higher order term $T - stress$ and the crack-tip speed in TAF1 sample. The error-bar corresponds to the sensibility to the extraction zone [Roux and Hild, 2006, Roux et al., 2009], the crack-tip speed v_c^o corresponds to the one reported in Figure 5.18 (computed from the crack opening)

crack-tips. The extraction become erroneous.

From Figure 5.8, the following observations can be drawn:

- From $t = 60\mu s$ (crack initiation from the notch) to $t = 95\mu s$, K_{ID} increases from $K_{ID} \simeq 2.68MPa\sqrt{m}$ to a plateau at $K_{ID} \simeq 6MPa\sqrt{m}$.
- The velocity of the elastic crack-tip on the other hand reaches a plateau around $v_c = 0.5c_R$ at $t = 70\mu s$, oscillations around this plateau are observed and the maximum velocity $v_c = 0.55c_R$ is reached at $90\mu s$. Afterwards, the crack-tip starts decelerating until it reaches $v_c \simeq 0.52c_R$ at the moment of branching, around $t = 95\mu s$.
- Regarding the first higher order term, knowingly the $T - stress$, an initial decrease is observed from $11MPa$ initially to a minimum of $T - stress = 2.46MPa$ at $t = 77\mu s$. Afterwards, $T - stress$ rockets through $T - stress = 13.46MPa$ at the moment of branching.

The rapid **increase of $T - stress$** before the crack branching echoes the tensile stress-wave reflected from the right-hand side boundary that was observed in Figure 5.6 and discussed

in Section 5.2.5. The increase of $T - stress$ before branching is also observed in TAF2, T3DE and THOM samples (Appendices G, H, I).

5.2.8 Experimental campaign summary

- Inertial impact test on a distinctive geometry allowing compelling crack propagation - stress-wave phenomena
- UHS-HR recording of the experiments and application of DIC to obtain full-field kinematic measurements

From here,

- Data processing of the DIC fields enables the rough description of the crack patterns and crack history
- Extraction of meaningful quantities relative to SIF directly from the DIC displacement fields

From DIC and the extractions, it's observed that:

- The hole of the specimen creates traction zones sideways
- The crack at the left-hand side of the hole is first initiated ($t = 40\mu s$)
- A second crack initiates from the notch at the right-hand side of the hole (at $t = 60\mu s$), with $K_{ID} = 2.68MPa\sqrt{m}$
- The crack accelerates to around velocity of $v_c = 0.55c_R$
- A plateau at $K_{ID} \simeq 6MPa\sqrt{m}$ is observed
- Tensile stress-waves parallel to the crack meet the crack-tip, the crack bifurcates into two branches at $v_c = 0.52r_R$ (at $t = 95\mu s$) with $K_{ID} = 6.45MPa\sqrt{m}$ and $T - stress = 13.46MPa$;
- The rapid increase of the $T - stress$ (extracted from the DIC displacement fields) reflects the tensile stress-waves meeting the crack (previous point).

We mainly focus on the last two points namely the branching and the role of the crack-tip speed and the increase of $T - stress$. We aim at **quantifying** the role that is played by a tensile stress parallel to the crack path (fancy name for $T - stress$) on the **crack instability and branching**. To do so, we propose a method to advocate the instability source at the branching position in the experiments.

First, we show how [Yoffe, 1951, Freund and Hutchinson, 1992]’s derivation regarding the angular variations of the circumferential tensile stress cannot explain the branching observed in this experiment, and more importantly, how building on [Ramulu and Kobayashi, 1983]’s work by adding higher order terms T – *stress* to the solution succeeds in yielding a change in the fracture direction and thus explains the instabilities and subsequent phenomena.

5.3 $\max(\sigma_{\theta\theta})$: a growth criterion

A multitude of criteria were proposed for crack extension and fracture [Cotterell and Rice, 1980, Erdogan and Sih, 1963, Hussain et al., 1974, Gupta, 1976, Palaniswamy and Knauss, 1978, Williams and Ewing, 1972]. The most fundamental ones assumes that the crack should advance in the direction that maximises the energy release rate [Hussain et al., 1974, Gupta, 1976, Palaniswamy and Knauss, 1978]. An alternative theory suggests that locally, the crack will choose the direction at which the local stress field at the tip is symmetric (similar to mode I , no mode II sliding). The **maximum circumferential tensile stress criterion** ($\sigma_{\theta\theta}$) is first proposed in quasi-statics by [Erdogan and Sih, 1963], and adopted in dynamics by many authors [Williams and Ewing, 1972, Streit and Finnie, 1980, Finnie and Saith, 1973]. Its success rests on its simplicity: **an analysis of the stress state near the crack-tip is sufficient to predict its extension behaviour.**

The maximum circumferential stress criterion in the vicinity of a moving crack-tip (v_c) has previously been analysed by considering the leading term ([Freund and Hutchinson, 1992, Yoffe, 1951]), i.e., SIF ; Figure 5.9(a) shows the variation of the maximum circumferential tensile stress with angle θ around the crack-tip for a material of Poisson ratio $\nu = 0.3$ for several values of normalised crack speeds v_c ([Freund and Hutchinson, 1992]). This feature was first observed by [Yoffe, 1951] 60 years ago.

Figure 5.9(b) shows the evolution of the direction of maximum circumferential stress $\sigma_{\theta\theta}$ that is computed as follows:

$$\theta_0(v_c) = \arg \max_{\theta} \sigma_{\theta\theta}(\theta, v_c), \text{ with } \sigma_{\theta\theta} > 0 \quad (5.1)$$

Consequently the circumferential stress reaches a maximum $\sigma_{\theta\theta}^0$ at a $\theta_0 \neq 0$ angle when the crack-tip speed exceeds a critical velocity threshold.

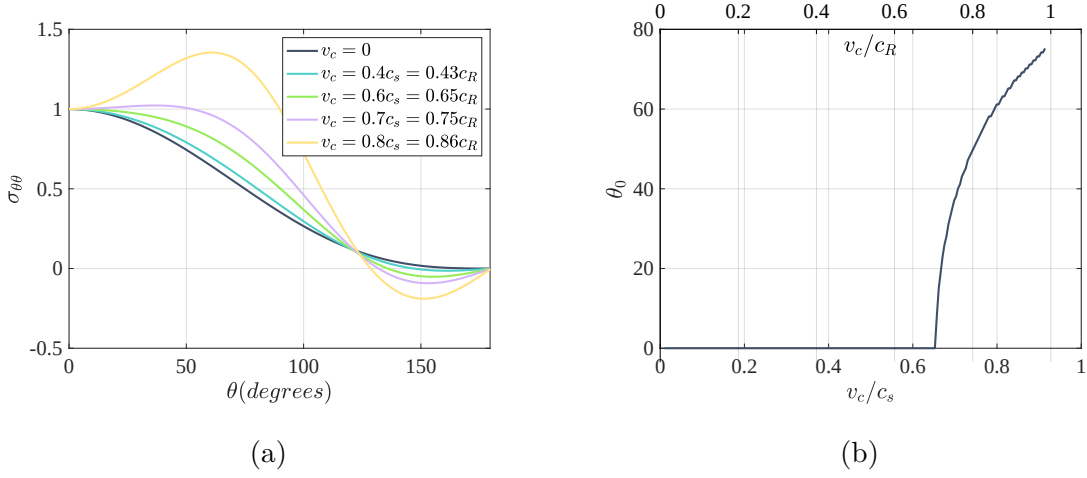


Figure 5.9 – Angular distribution of $(\sigma_{\theta\theta})$ at different v_c [Yoffe, 1951] (a), and the direction θ_0 of $\sigma_{\theta\theta}^0 = \max \sigma_{\theta\theta}$ as a function of the normalised crack-tip speed (b)

But how does the angular distribution of the stresses relate to crack instabilities relate to branching?

As the crack-tip speeds increase (see Figure 5.9), the direction of maximum $\sigma_{\theta\theta}$ stays primarily in the extension of the crack growth, however, a sort of plateau is reached around a crack-tip speed of $v_c = 0.7c_R$; this suggests a homogenisation of the maximum stress along multiple critical directions. Essentially, as a result of the crack-tip fields, the coalescence of micro-defects in the vicinity of the tip leads to crack growth in a direction close to **any direction** of maximum $\sigma_{\theta\theta}^0$ this translates to what is known as **directional instability**. At higher crack-tip speeds, the plateau vanishes and the directional instability is mainly bounded to the two symmetric directions $\pm\theta_0$ of maximum $\sigma_{\theta\theta}$, which yields branching.

Although this derivation was able to predict that the limiting velocity for a stable crack is lower than c_R , unfortunately, this cannot explain the lower critical velocities observed in the experiments.

5.3.1 Experimental assessment of the instability: classical solution

In this inertial impact test previously presented, the crack reaches a top speed of $0.55c_R$ yet bifurcation occurs at $0.52c_R$. The theory of dynamic fracture mechanics characterises

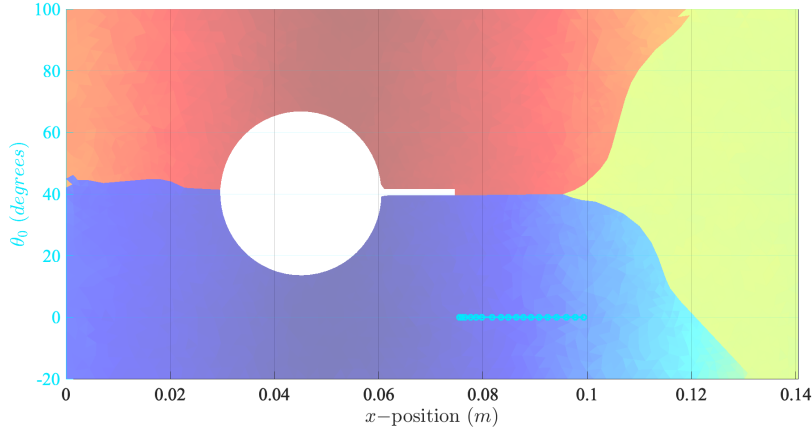


Figure 5.10 – Evolution of the predicted fracture direction θ_0 from the classical solution (experimental SIF and v_c). The branching is not reflected in the criterion

the stress state near the crack front for a linear elastic isotropic material Chapter 0. Assuming that the PMMA sample is a linear elastic isotropic material (Subsection 5.2.7, Table 5.1), the experimentally determined crack-tip velocities v_c and K_{ID} (no $T - stress$) are injected into the elastodynamics solution of the stress-field in the vicinity of the moving crack-tip. The fracture direction $\pm\theta_0$ is subsequently computed for each frame of the advancing crack, based on the criterion of maximum circumferential stress. The scheme of analysis is summarised as follows:

$$\underline{u}_{DIC} \rightarrow SIF, \text{ crack-tip position and } v_c \rightarrow \underline{\sigma} \rightarrow \sigma_{\theta\theta} \rightarrow \sigma_{\theta\theta}^0 \ \& \ \theta_0$$

where $\sigma_{\theta\theta}$ corresponds to the circumferential stress which maximum value $\sigma_{\theta\theta}^0$ is along the fracture angle (propagation direction) θ_0 .

From here, the evolution of the direction $\pm\theta_0$ at different positions of the crack-tip inside the material is reported in Figure 5.10. A criterion should be able to reproduce a modification in the direction of propagation at the branching position. Observing the obtained trend of θ_0 , it's clear how the fracture direction is always along the crack growth, even at the branching position.

As it is, this criterion fails to assess the crack (in)stability. The same exercise is repeated in the next section, but this time by considering the higher order term $T - stress$ from the experimental estimation to the solution.

5.4 Incorporating $T - stress$

The same exercise (injecting experimental SIF and crack-tip speeds in the asymptotic solution of the stress fields and determining the directions of maximum circumferential stress at each position of the crack) is repeated in this section under one modification: adding the first non-singular term $T - stress$ to the stress solution. First we recall one foundation of LEFM and we evoke the need for higher-order terms in the asymptotic solutions as they play a major role in fracture (static crack path stability, isochromatic fringes pattern, plastic zone influence, etc.) [Gupta et al., 2015]. [Ramulu and Kobayashi, 1983, Ramulu and Kobayashi, 1985]’s criterion is recalled and is built upon for accurately addressing the instabilities.

LEFM and its dynamic counterpart are found around the notion of small-scale yielding. The small scale yielding incorporates the notion that the leading SIF terms still govern the deformation state inside a fracture process zone at the crack-tip. However, it is becoming more recognised that non-singular stresses can become significant depending on the geometry and loading of the specimen, and the role of $T - stress$ for example has been extensively studied [Gupta et al., 2015], especially in quasi-static.

When incorporating higher order terms, it’s assumed that fracture growth occurs at a given distance r_c ahead of the crack-tip where the contribution of the higher-order terms become significant to the fracture process. Beyond enabling the assessment of higher-order terms, the assumption of such given distance was shown to be physically reasonable by many authors [Rice, 1970, Ritchie et al., 1973, Streit and Finnie, 1980] arguing that r_c corresponds to a distance from a crack-tip at which micro-defects can coalesce as an extension of the crack. Of course, this r_c would depend on each materials’ heterogeneities at the microscopic levels.

When adding the $T - stress$ to the stress solution, Equation 5.1 can be rewritten as at any distance r from the crack-tip:

$$\theta_0(r, v_c, T) = \underset{\theta}{\operatorname{argmax}} \sigma_{\theta\theta}(r, \theta, v_c, T, K_{ID}), \text{ with } \sigma_{\theta\theta} > 0 \quad (5.2)$$

and when analysing crack growth, $r = r_c$ is set to assess the relevant angular distribution of the stresses at the distance from the tip at which a crack would grow.

Within this context, [Ramulu and Kobayashi, 1983] proposed a criterion that predicts the instabilities for crack-tip speeds $v_c < 0.67c_s = 0.72c_R$ ⁶ based on the introduction of a

6. The classical solution (without non-singular terms) would give stable crack propagation ($\theta_0 = 0$) in

reference distance scale r_o that is a function of $T - stress$, K_{ID} and the crack-tip speed v_c . r_o represents a distance below which the crack propagation is dominated by the SIF , i.e., the direction of propagation is along the extension of the crack, which means that the directional stability of a mode I propagating crack is maintained. For a material of critical distance r_c , the stability condition requires r_c to be in a SIF -dominated zone, i.e., $r_c \leq r_o$. Interested readers are referred to the following subsection for more details about [Ramulu and Kobayashi, 1983]’s criterion, incidentally skipping the next subsection does not affect the overall flow. Our derivations are pursued in Section 5.4.1.

Computation and significance of r_o

From the elastodynamics solution and Equation 5.2, by finding the expression of θ_0 , and setting it to zero (stable), a sufficient condition for stability emerges as a function of K_I , $T - stress$, and the crack velocity v_c . Indeed, the crack propagation is considered stable when it tends to propagate along its direction of growth, i.e., at $\theta_0 = 0$. This condition brings forth a unique reference distance $r = r_o$ as a function of K_{ID} , $T - stress$ and the crack velocity v_c , valid in $0 \leq v_c \leq 0.67c_s = 0.72c_R$:

$$r_o = \frac{1}{128\pi} \left[\left(\frac{K_{ID}}{\sigma_{0x}} \right) V_0(v_c, c_d, c_s) \right]^2 \quad (5.3)$$

where V_0 is defined as:

$$\begin{aligned} V_0(v_c, c_d, c_s) = & B_d(v_c) \left(-(1 + S_s^2)(2 - 3S_d^2) \right. \\ & \left. - \frac{4S_d S_s}{1 + S_s^2} (14 + 3S_s^2) - 16S_d(S_d - S_s) + 16(1 + S_d^2) \right) \end{aligned} \quad (5.4)$$

where

$$\begin{aligned} B_d(v_c) &= \frac{1 + S_s^2}{4S_d S_s - (1 + S_s^2)^2} \\ S_d^2 &= 1 - \frac{v_c^2}{c_d^2} \\ S_s^2 &= 1 - \frac{v_c^2}{c_s^2} \end{aligned} \quad (5.5)$$

this range of crack-tip speeds $0 \leq v_c \leq 0.67c_s = 0.72c_R$

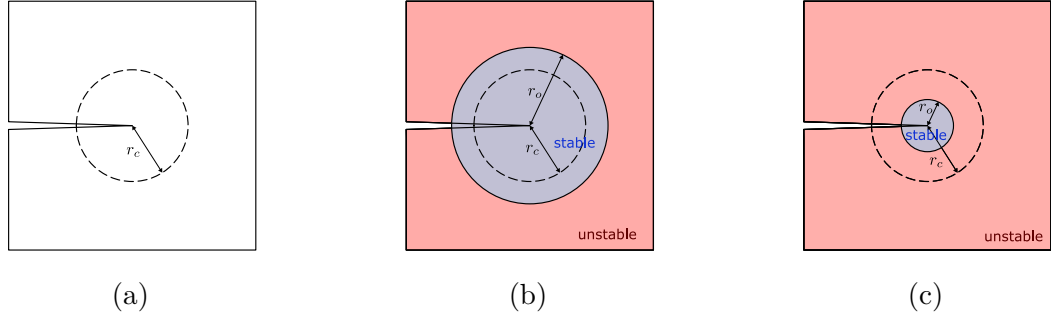


Figure 5.11 – The stability criterion $r_o \geq r_c$. r_c is a material parameter stating the distance at which damage may occur. r_o can be seen as a representation of the stress field. In $r \leq r_o$, a K -dominant zone is omnipresent. The criterion stands for $0 \leq v_c \leq 0.67c_s = 0.72c_R$

σ_{0x} is equivalent to $T - stress$, i.e., a far-field stress acting parallel to the direction of crack extension.

The sufficient **stability** condition relating the material critical distance r_c to the (in)stability reference distance r_o reads:

$$r_o \geq r_c \quad (5.6)$$

Figure 5.11 shows a schematic representation of the criterion. Stable and an unstable cases are shown, based on [Ramulu and Kobayashi, 1983]’s criterion. The red zone corresponds to a zone where K is not dominant, and far-field stresses play a major role in determining the angular distribution of the crack direction. The blue zone corresponds to the stability zone, in which K is dominant.

For an **arbitrary** material of critical crack growth distance r_c , Figure 5.12 shows the evolution of r_o at fixed $T - stress$ as a function of the crack-tip speeds. It also shows the influence of $T - stress$ on r_o at two fixed speeds (one comparable to a quasi-static propagation and another one at $v_c = 0.5c_R$). As Equation 5.6 states the stability condition being $r_o \geq r_c$, in Figure 5.12(a), this translates to an unstable crack growth for a crack starting $v_c \simeq 0.68c_R$ - for the considered arbitrary material, under an arbitrary $T - stress$. Of course, $T - stress = 0$ would yield an ever-stable crack under this criterion (within its range of application $0 \leq 0.67c_s = 0.72c_R$), coherently with the classical solution [Yoffe, 1951].

In Figure 5.12(b), [Ramulu and Kobayashi, 1983]’s criterion predicts unstable crack propagation even under negative $T - stress$ at low crack-tip speeds, which is in contradiction with multiple works (see e.g., [Gupta et al., 2015] for a review of the influence of $T - stress$

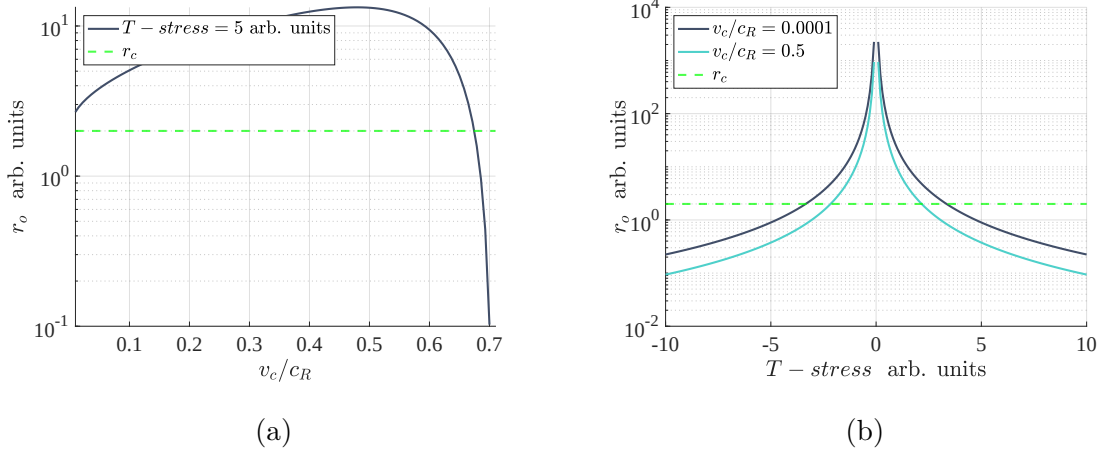


Figure 5.12 – The stability criterion $r_o \geq r_c$. Influence of the crack-tip speeds (a) and the $T - stress$ (b). At $T - stress = 0$, the criterion gives an ever-stable crack (in the range $0 \leq 0.67c_s = 0.72c_R$, coherently with the classical solution [Yoffe, 1951])

on crack propagation). Moreover, it's evident how a faster running crack (e.g., $v_c = 0.5c_R$ versus $v_c = 1e^{-4}c_R$) is more prone to instabilities at lower $T - stress$ levels.

Further, this criterion suffers from some limitations:

- The inability to incorporate branching at fast running cracks from the classical solution, for example, under complex stress-wave propagation and reflection, $T - stress$ would be extremely volatile and building a criterion that is able to predict instabilities in the absence and presence of $T - stress$ is crucial;
- Prediction of crack instability at negative $T - stress$ under near quasi-static loading, which was contradicted by various authors [Gupta et al., 2015].

Remark 5.10. In [Ramulu and Kobayashi, 1983, Ramulu and Kobayashi, 1985]'s work, the determination of the critical distance r_c is made across multiple experiments by determining r_o^{inst} , which is the value of r_o just before the instability, and noting $r_c = r_o^{inst}$. In the 1980s, the ability to estimate highly resolved (in time) SIF, $T - stress$ and crack-tip speeds experimentally was lacking, so r_c was considered as the smallest r_o computed across the experiments. With the advancement in ultra-high speed imaging and DIC procedures, we believe that a more accurate identification of r_c hence a more accurate criterion can be obtained.

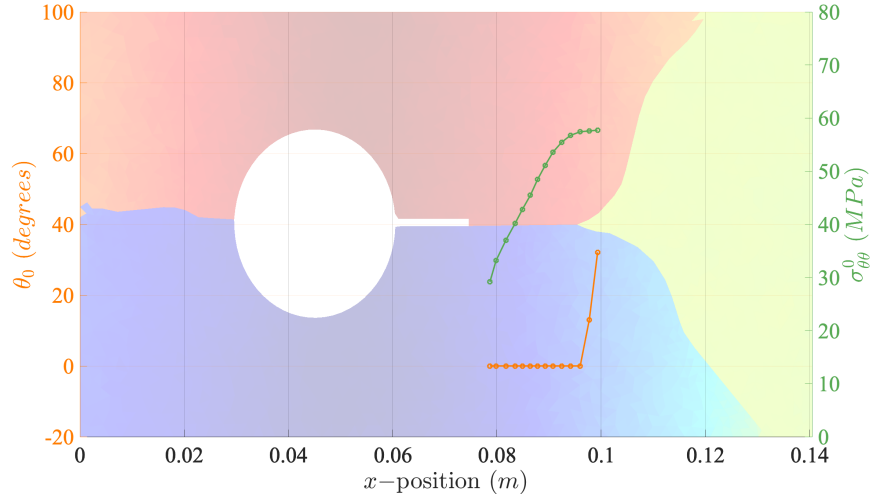


Figure 5.13 – Evolution of the predicted fracture direction θ_0 along with the maximum circumferential stress computed at $r_c = 2mm$ in TAF1 sample (SIF , $T - stress$ and v_c from DIC experimental fields). The modification of the fracture angle θ_0 at the position of branching and the evolution of $\sigma_{\theta\theta}^0$ mirror the experimental branching.

5.4.1 Application to the inertial impact test

Back to the experiments now, since the DIC provides good estimates of the frame ($\pm$ one frame) at which the branching occurs, the sample's critical distance r_c can be obtained by computing r_o^{inst} as being r_o at the branching frame, and setting the (in)stability condition $r_c = r_o^{inst}$. Since $r_c = r_o$ preconises the limit of instability, one can foresee that for any $r_o \geq r_o^{inst} = r_c$, the propagation is also unstable so $r_c = r_o^{inst}$ should be a first candidate at estimating r_c . r_c can then be manually optimised (trial and error) to accurately reproduce the experimental branching angles.

The critical value $r_c = 2 \pm 0.16mm$ is consistently found across the four experiments, which proves it to be a material constant as previously preconised [Rice, 1970, Ritchie et al., 1973, Ramulu and Kobayashi, 1983]. The identification is directly obtained from $r_c = r_o^{inst}$ without manual optimisation.

Experiment assessment of the instability: incorporating $T - stress$

The evolution of the direction $\pm\theta_0$ at different positions of the crack-tip inside the material is reported in Figure 5.13.

Observing the obtained trend of θ_0 , it's clear how:

- the fracture direction is always along the crack growth along the crack propagation from the notch till before the branching position;
 - at the branching position, the direction of propagation is accurately predicted by the change of θ_0 (increase from $\theta_0 \simeq \pm 0$ to $\pm 10^\circ$ to $\pm 32^\circ$);
 - $\sigma_{\theta\theta}$ increases and reaches a plateau around $55MPa$ before branching.
-

General results of the four samples

The following observations are drawn from analysis of the samples TAF1, TAF2, T3DE and THOM:

- For the 4 samples, the maximum circumferential stress before branching reaches $55MPa \pm 8MPa$.
- The branching angles are reflected on the change in the direction of fracture θ_0 at the branching position; at velocities around $v_c = 0.52c_R$ for TAF1 and T3DE, and around $v_c = 0.4c_R$ for TAF2 and THOM.
- $r_c = 2 \pm 0.16mm$ is consistently found across the four experiments.

Hence the unquestionable role played by $T - stress$ on the branching instability at relatively low crack-tip speeds ($v_c = 0.4 - 0.52c_R$) is highlighted via simple fracture mechanics concepts combined with advanced imaging and experimental technologies.

5.5 The (in)stability map: a comprehensive criterion

After putting-forth the unquestionable role of $T - stress$ on crack (in)stability, we wrap-up this experiential study by constructing a comprehensive (in)stability criterion called the **material (in)stability map**. It is built based on experimental findings. It is a map that embodies a criterion for the transition between stable and unstable crack propagation for crack-tip speeds $0 \leq v_c \leq c_R$ with the unquestionable role of $T - stress$ at its core. The goal is to determine, for a given material (knowing its density ρ , its elastic properties E , ν , its fracture toughness K_{IDC} - or crack propagation behaviour - , **and** its material constant r_c) the loadings (in terms of fracture mechanics, i.e., K_{ID} , $T - stress$, v_c) under which crack growth is stable and the loadings under which crack growth is not.

We proceed as follows: as it's assumed that fracture is driven by the stress field in the local neighbourhood, **we sweep a large range of $T - stress$ and crack-tip speeds**

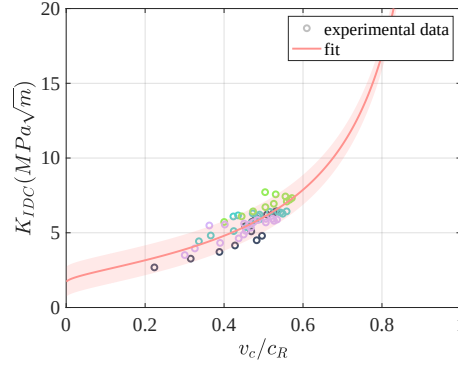


Figure 5.14 – Experimental K_{ID} and v_c (circular markers) with the fit corresponding to the crack propagation behaviour law following [Kanninen and Popelar, 1985] $K_{IC} = 1.66 \text{ MPa}\sqrt{\text{m}}$ and $m = 0.465$ are found, the colours corresponds to experimental data from the different samples

and find the direction θ_0 of maximum circumferential stress $\sigma_{\theta\theta}^0$ at distance r_c from the crack-tip. This allows the construction of a 2D surface that gives θ_0 and $\sigma_{\theta\theta}^0$ as a function of a crack-tip speed v_c and T – stress. The construction is as follows:

- the materials elastic properties are experimentally determined via the in-house FEMU (Subsection 5.2.7) and reported in Table 5.1;
- the material constant r_c is experimentally computed from the application of [Ramulu and Kobayashi, 1983]’s criterion on SIF , T – stress and v_c information from full-field measurements
- The full-field measurements provide SIF and v_c data on the relationship between the stress intensity factor and the velocity of the crack-tip. Assuming that the crack advances at $K_{IDC} = K_{ID}$, where K_{ID} is the instantaneous dynamic stress intensity factor estimated from full-field measurements, it’s found that the empiric law proposed by [Kanninen and Popelar, 1985] Equation 5.7 relating the critical dynamic stress intensity factor K_{IDC} , to its static counterpart K_{IC} and the eventual crack-tip speed fits well the experimental data:

$$K_{IDC} = \frac{K_{IC}}{1 - \left(\frac{v_c}{c_R}\right)^m} \quad (5.7)$$

where K_{IC} is the static counterpart of the fracture toughness and m is a material constant.

Figure 5.14 shows the behaviour law of the crack propagation fitted on data from the

4 samples. The determined parameters $K_{IC} = 1.66 \text{ MPa}\sqrt{\text{m}}$ and $m = 0.465$ accurately portray the dynamic crack propagation behaviour in the PMMA samples.

Having all the required information, the material (in)stability map is constructed and showcased in Figure 5.15(a) in the $(v_c, T - \text{stress})$ space. We analyse an arbitrary range of $T - \text{stress}$ between -30 MPa and $+30 \text{ MPa}$. Figure 5.15(b) shows the equivalence in the $(K_{ID}, T - \text{stress})$ space. In this range of $T - \text{stress}$, 5.15(a), one can observe the following:

- At $T - \text{stress} = 0$, the classical solution is recovered (Figure 5.9(b))
- For crack-tip speeds $0 \leq v_c \leq 0.8c_R$, a negative $T - \text{stress}$ stabilises the crack.
- Even at slow crack-tip speeds, e.g., $v_c = 0.05c_R$, the presence of a $T - \text{stress}$ can foster instabilities and eventual branching.
- Above $v_c = 0.8c_R$, independently of the values of $T - \text{stress}$, instability is prominent.
- Dependently of the intensity of tensile stress along the direction of the crack ($T - \text{stress}$), different limiting velocities can be reached.
- The sharpness of the transition zone between the stable and unstable crack growth varies with the crack-tip speed and $T - \text{stress}$. Since we do not have access to accurate SIF , $T - \text{stress}$ and crack-tip speeds after branching, and since our temporal discretisation is not fine enough to register more data points around the branching, we are restricted from further investigating the smoothening/sharpening of the transition zone. But we believe that a more careful inspection is required to understand the sharp/smooth transition on the crack instability.

Remark 5.11. *These observations only stand for the (in)stability map herein considered, i.e., for the PMMA, of course each material would have a different (in)stability map, e.g., a material with the same mechanical properties as PMMA, but which critical distance r_c is much bigger than 2mm would withstand even less $T - \text{stress}$ at stable propagation, since more weight would be given on the higher-order terms. Follow up in Appendix J where the influence of r_c on the (in)stability map of an arbitrary material is highlighted for demonstration purposes. Obtained results can be generalised.*

Remark 5.12. *A commonly used scheme to ensure directional stability at high crack-tip speeds is to side groove the test pieces. This would normally allow the cracks to reach near-sonic crack-tip speeds. Regarding the fact that the (in)stability map Figure 5.15(a) shows a limiting velocity always smaller than c_R , in the case of a side-groove, complex*

state of stress on the specimen that cannot be taken into account in the (in)stability map are created. So this side grooving exercise is out of the scope of this study.

In Figure 5.15(b), one can especially observe the broadening of the transition zone with the increase in K_{IDC} . It's mentioned that $K_{IDC} = 10MPa\sqrt{m}$ corresponds to a crack-tip speed $v_c = 0.672c_S = 0.72c_R$ so the broadening of the transitional zone is also recovered in the previous figure, as normal.

5.5.1 Experimental crack growth

The history of the crack propagation from the notch until its branching for the 4 samples are displayed on both Figures 5.15(a) and 5.15(b). The circular marker on the curves corresponds to the (frame ± 1 frame) at which the crack initiates from the notch (usually most south-west point in these experiments) and the arrowhead corresponds to the frame at which the crack branches (± 1 frame) (usually most north-east point in these experiments) .

In the $(v_c, T - stress)$ space (Figure 5.15(a)), the 4 growth patterns are similar, where a decrease in $T - stress$ with an accelerating crack are observed followed by a increase in $T - stress$. Two different crack propagation behaviours are observed for two couples of samples:

- the cracks TAF1 and T3DE branch at $v_c = 0.52 \pm 2e^{-4}c_R$ in the presence of a $T - stress = 14.23 \pm 1MPa$
- the cracks TAF2 and THOM branch at lower crack-tip speeds $v_c = 0.41 \pm 0.1c_R$, in the presence of a $T - stress = 13.46 \pm 0.3MPa$

The transition from the stable zone to the unstable zone coincides well with the branching position.

In the $(K_{IDC}, T - stress)$ space (Figure 5.15(b)), the 4 growth patterns are similar, where a decrease in $T - stress$ with an increase in K_{ID} are observed followed by a increase in $T - stress$, reflecting well the stress-waves 'seen' by the moving crack-tip. Two different crack propagation behaviours are observed for two couples of samples:

- a plateau (in K_{ID}) reached for TAF1 and T3DE; while
- a small decrease in K_{ID} is observed for TAF2 and THOM.
- the branching (equivalently the transition from the stable to the unstable zone in the map) occurs at $K_{ID} = 6.45, 6, 7.8$ and $5.51MPa\sqrt{m}$ for TAF1, TAF2, T3DE and THOM respectively.

Remark 5.13. *The similarity in the crack scenarios (by pair) is probably due to the fact that the impact velocities (Section 5.2.4) are similar for TAF1 and T3DE ($V_{proj} = 30.5\text{m/s}$ and 31.8m/s) from one side, and for TAF2 and THOM from the other ($V_{proj} = 22\text{m/s}$).*

The transition from the stable zone to the unstable zone coincides well with the branching position. An increase in K_{ID} does not necessarily foster branching as we’ve seen in some cases branching occurs at a plateau of K_{ID} , and others at a slight drop in this value. So K_{ID} reaching a certain critical value is a necessary condition, while the change of the fracture direction θ_0 is a sufficient condition.

We plot in Figure 5.16 the evolution of the maximum circumferential stress, i.e., along the direction θ_0 in the $(v_c, T - stress)$ and the $(K_{IDC}, T - stress)$ spaces. From Figure 5.16, one observes that the maximum value of $\sigma_{\theta\theta}^0$ does not necessarily account for crack branching as one would expect (the maximum value of $\sigma_{\theta\theta}^0$ is reached prior to the branching moment, i.e., before the arrowhead). In fact, as long as the crack propagation direction is $\theta_0 = 0$, the maximum stress (whatever its value) is along the extension of the crack, stabilising thus the propagation. However, if the crack direction diverges from the direction of the extension of the crack, instabilities and eventual branching occur. The deviation from $\theta_0 = 0$ is hence a sufficient condition to foster the instabilities, while the stress value is a necessary condition.

5.6 Discussion on the (in)stability map

The material (in)stability as presented here constitutes a great tool for understanding causes of crack instabilities and limiting velocities. Here we present a summary around it:

- The (in)stability map is constructed from highly resolved experimental full-field measurements recorded at ultra-high speeds.
- It constitutes a straightforward visual tool for assessing crack (in)stabilities, based on the crack-tip speed v_c and the presence of higher order terms ($T - stress$).
- In a 2D space $(v_c, T - stress)$ or $(K_{IDC}, T - stress)$, a surface representing the fracture angles divides the space into stable and unstable crack growth zones.
- The map shows how $T - stress$ ’ role is prominent on limiting the velocity of stable growth, and on crack (in)stabilities at low crack-tip speeds
- For $T - stress \leq 0$, the classical solutions are recovered and the crack-tip speeds control the (in)stabilities. No length-scale effect is observed (the angular distribution

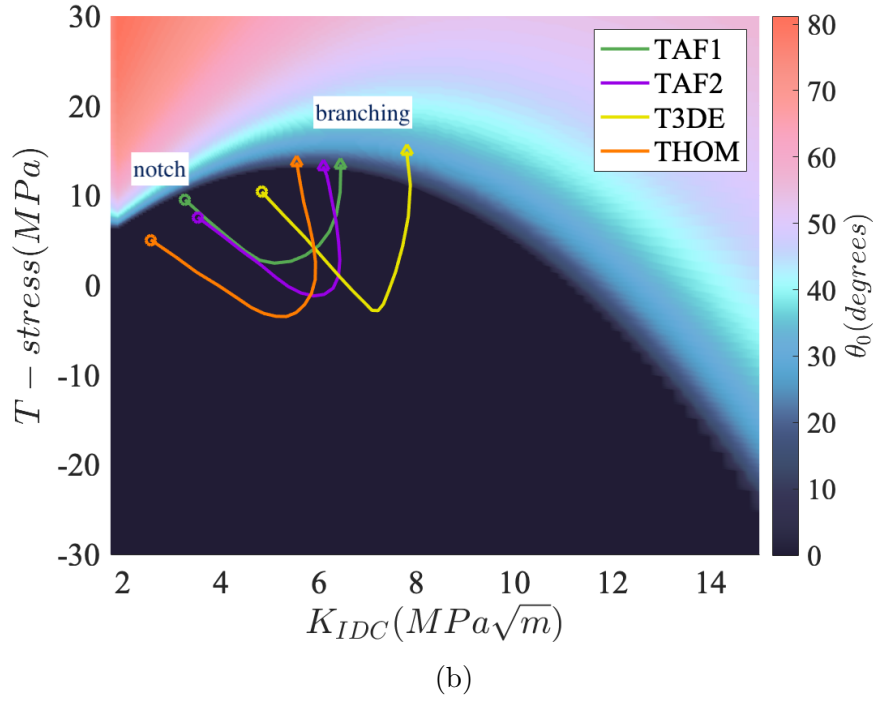
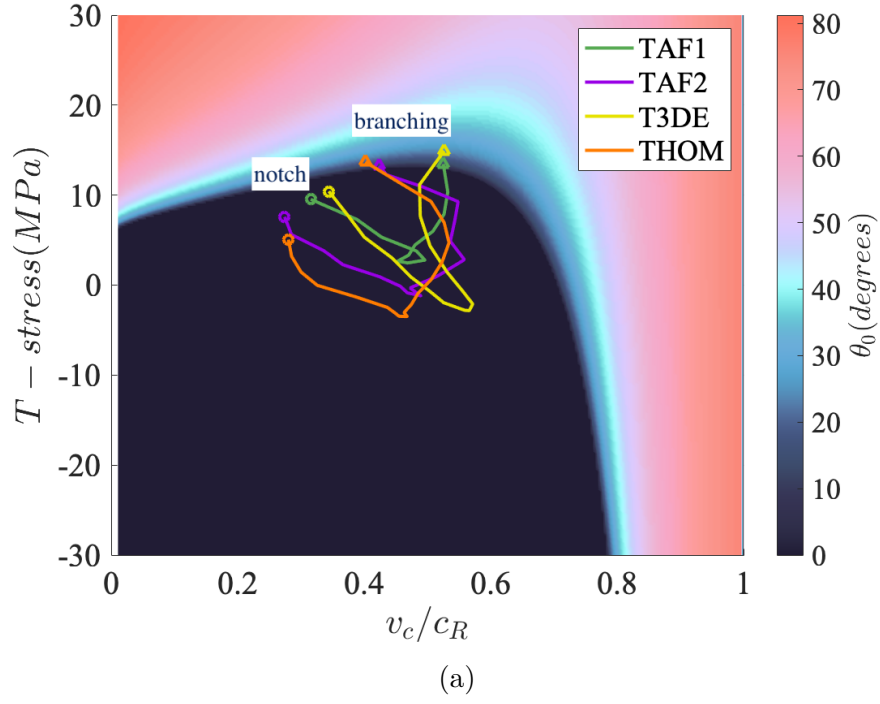


Figure 5.15 – (In)stability map of PMMA, constructed from experimental measurements and fitted to [Kanninen and Popelar, 1985]’s empiric law. The history of the crack propagation in each sample is displayed; from the initiation at the notch (circular marker) until the branching position (upward-pointing arrow) ± 1 frame, the map accurately predicts the (in)stability at the branching position with the change of θ_0

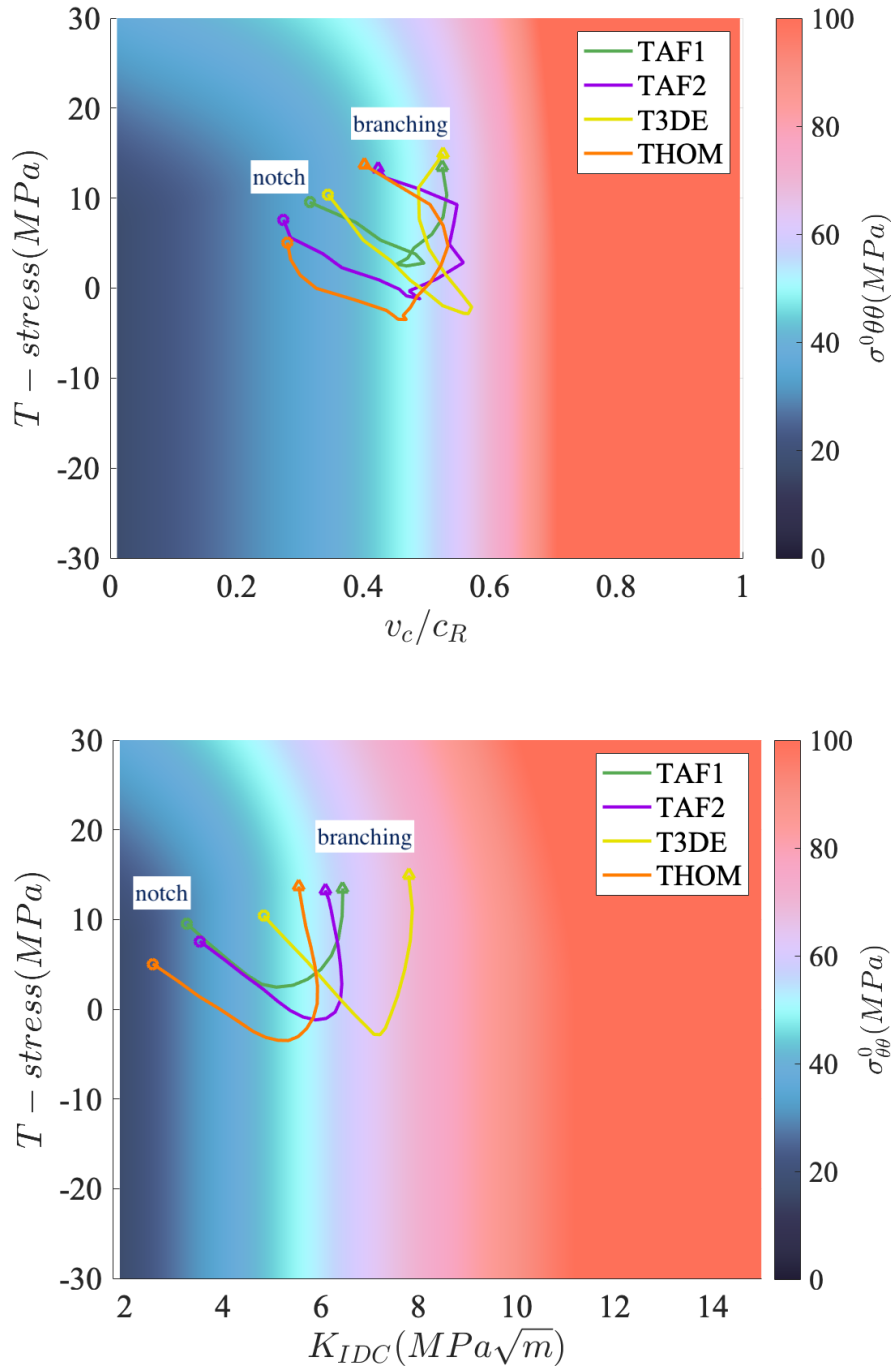


Figure 5.16 – Maximum circumferential stress map of the PMMA samples, constructed from experimental measurements and fitted to [Kanninen and Popelar, 1985]’s empiric law. The history of the crack propagation in each sample is displayed; from the initiation at the notch (circular marker) until the branching position (upward-pointing arrow) ± 1 frame

is conserved at different distances from the crack-tip)

- With $T - stress \leq 0$, r_c cannot be computed from [Ramulu and Kobayashi, 1983], hence if one were to determine r_c for a certain material, alternate experimental configurations should be considered, i.e., in which positive $T - stress$ is present and in which an unstable crack is present.
- In the presence of $T - stress$, the material critical distance r_c plays a major role in the crack growth. Accurately assessing r_c is crucial for crack angle predictions
- The transition zone between stable and unstable crack growth is well defined, however, its sharpness seems to depend on both $T - stress$ and the crack-tip speed v_c .
- Of course, we couldn't cover the ever-growing wide range of dynamic configurations, and many crack branching scenarios have not been explored. However, never have we ever been able to extract such meaningful information as we did from a brisk $200\mu s$ -long (short) test. We believe that the ability to experimentally assess crack (in)stabilities via the proposed analysis is an ambitious finding in quest for further understanding the rich dynamic phenomena.

5.7 A phase-field simulation of the inertial impact test

After successfully assessing the role played by $T - stress$ on crack (in)stabilities, we check the ability of the phase-field model to replicate the experimental crack propagation in the inertial impact test (Section 5.2). More prominently, we apply the analysis scheme on the simulation displacement fields to further elaborate on the mechanisms of branching in the phase-field models. A detailed version of this section is available in Appendix K for interested readers.

We briefly recall the ingredients of the phase-field model used, and the material properties that allowed a loyal reproduction of the crack paths:

5.7.1 On the crack patterns

Figure 5.17 shows both experimental (*DIC* measurements) and simulation results (phase-field simulations) of the inertia impact test TAF1. The crack patterns are clearly

Time stepping	Explicit ([Li et al., 2016b])
Crack density function	Quadratic (Equation 1.3) ([Miehe et al., 2010a])
Strain split	Orthogonal ([Nguyen et al., 2020b])
Plane strain assumption	
Boundary condition	Experimental <u>u</u> [Vinel et al., 2021], check Appendix K
E (Young's Modulus)	6GPa , previously addressed in Section 5.2.7
ν	0.3, previously addressed in Section 5.2.7
g_c	1100J/m ²
l_c	2× mesh size = $2 \times h = 1mm$ ([Nguyen et al., 2016])
c (threshold)	1

Table 5.2 – Overall phase-field model and material parameters considered in this simulation of the inertial impact test.

reproduced by the phase-field simulation: the branching position and the branch turning are accurately predicted.

We note the widening of the damage band in the simulation before the moment of branching, similarly to other phase-field simulations reported in [Borden et al., 2012], [Schlüter et al., 2014], and to non-local integral damage model [Pereira et al., 2017]⁷. To further investigate the branching and damage band widening, the (in)stability criterion is applied. Beforehand, let us briefly describe the crack path history and crack-tip speeds from the simulation and compare them with the experimental results from *DIC*.

5.7.2 On the crack-tip speeds

In Figure 5.18, we superpose the crack-tip velocities from the simulation and the crack-tip velocities obtained experimentally. Even though the crack patterns are accurately reproduced, the crack path history and crack-tip speeds are not.

This can be caused by various reasons, possibly and not exclusively;

- Viscous effects: even though PMMA is THE model material for in-lab studying the brittle elastic failure, its viscous behaviour has already been documented and quantified, e.g., in [Seghir and Pierron, 2018].

7. From a more physical point of view, damage widening could be the signature of roughening of the crack surface experimentally observed to occur prior to branching [Ramulu and Kobayashi, 1985]. [Bleyer and Molinari, 2017] showed that the micro-branching process is indeed a three-dimensional instability and is directly linked to surface patterns observed prior to macro-branching in PMMA [Sharon and Fineberg, 1996].

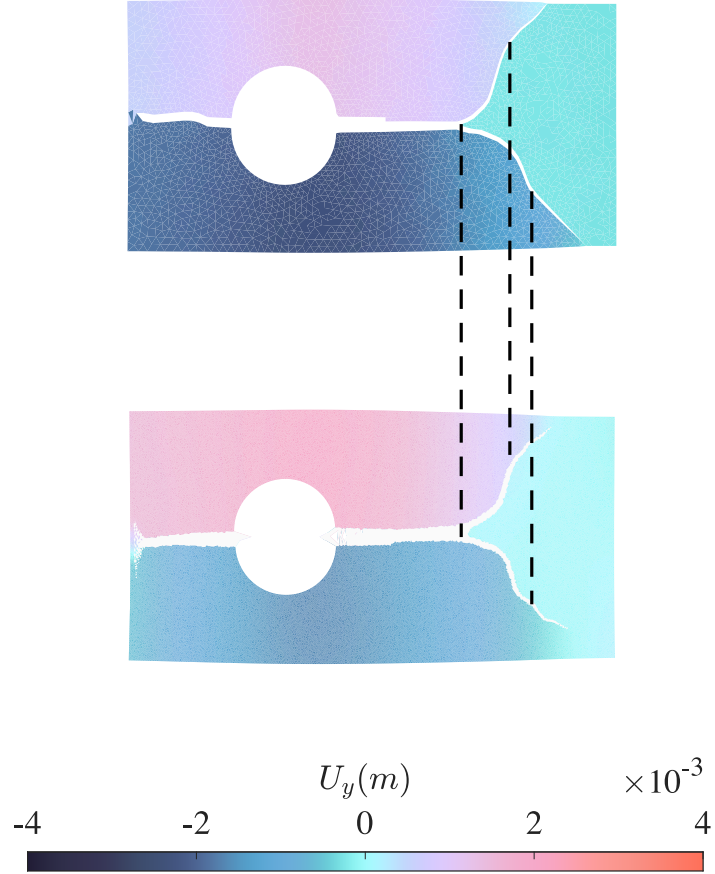


Figure 5.17 – *DIC* displacement field (up) and phase-field simulation results (down) showing accurate prediction validating the dynamic phase-field model and accurately reproducing the crack patterns. The points where the phase-field damage $\alpha \geq 0.99$ are removed to mimic crack opening.

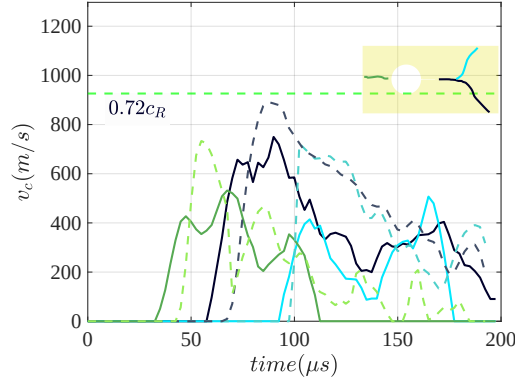


Figure 5.18 – Comparison of the experimental and numerical (phase-field simulation) crack-tip speeds. Dashed lines correspond to the crack-tip speeds estimated from the phase-field simulation (Appendix B), full lines correspond to the apparent experimental crack-tip-speeds previously reported in Figure 5.7 (computed from crack opening)

- Wrong phase-field parameters: as seen in Chapter 1 and Appendix A, comparable crack paths can be obtained for different combinations of parameters l_c , g_c and c , however, discrepancy in the crack-tip speeds are often present. With the contribution to the phase-field modelling in Chapter 1, the parametrisation of the threshold (Chapter 1) allows for a triplet of parameters to be optimised for accurately reproducing experimental scenarios by elegantly balancing the energy dissipation, energy release-rate and fracture strength. This yields more freedom in the choice. Even though this parametrisation offers a wider range of material behaviour, it is crucial to span the triplets in the search for the optimum phase space.

Remark 5.14. *Without the UHS-HR imaging and the cutting edge DIC algorithms, the obtained simulation results would be satisfactory. However, these technological advancements offer sound ground for a more rigorous estimation of the phase-field parameters that should yield a more precise reproduction not only of the patterns, but also crack-tip speeds and crack history.*

Next, we advocate instabilities on the phase-field simulation results based on the proposed method.

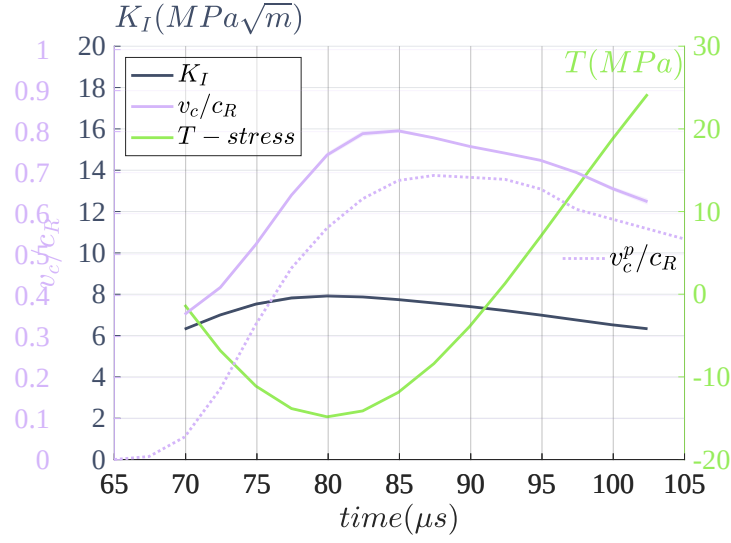


Figure 5.19 – *SIF*, the higher order term *T – stress* and the crack-tip speed in the simulation of the TAF1 sample test. The error-bar corresponds to the sensibility to the extraction zone [Roux and Hild, 2006, Roux et al., 2009]. The crack-tip speed v_c^p corresponds to the one reported in Figure 5.18 computed from the phase-field, via Appendix B

5.7.3 Crack branching analysis

Indeed, since only displacement fields are required for the analysis, the proposed scheme is readily applicable on displacement fields coming from numerical simulations.

$$\underline{u}_{SIMU} \rightarrow SIF, T - stress, \text{ crack-tip position, and } v_c \rightarrow \underline{\sigma} \rightarrow \sigma_{\theta\theta} \rightarrow \sigma_{\theta\theta}^0 \ \& \ \theta_0$$

Figure 5.19 shows the estimations of the crack-tip speed, *SIF* and *T – stress*; the following observations can be drawn:

- The estimations show similar trends to the experimental estimations.
- From $t = 70\mu s$ (crack initiation from the notch) to $t = 80\mu s$, K_{ID} increases from $K_{ID} = 6.28 MPa\sqrt{m}$ to $K_{ID} = 7.91 MPa\sqrt{m}$.
- The velocity of the elastic crack-tip on the other hand reaches a maximum $v_c = 0.8c_R$ at $t = 85\mu s$. Afterwards, the crack-tip starts decelerating until it reaches $v_c \simeq 0.72c_R$ at the moment of branching (branching detected from Figure 5.18), around $t = 95\mu s$.

Remark 5.15. *On the difference between the computed crack-tip speeds: the phase-field model introduces a damaged zone in which the dissipative processes are diffused to regularise a sharp crack (via the length-scale l_c). The methodology proposed in Appendix D is founded on LEFM that suggests that all non-linear and dissipative processes are well confined to the near-tip vicinity. The equivalent elastic crack-tip (extracted from Appendix D) would eventually not coincide with a phenomenologically captured crack-tip (e.g., iso-curves of the phase-field), the equivalent elastic crack-tip is expected to accelerate as the damage band widens/lengthens and dissipates energy. A delay/deviation between those two computed speeds is natural as it comes from their inherent differences.*

- Regarding the first higher order term, knowingly the $T - stress$, an initial decrease is observed to a negative $T - stress = -15MPa$ at $t = 80\mu s$. Afterwards, $T - stress$ rockets.
- As mentioned in Remark 5.2, neat imaging could not be achieved. Despite the application of the novel calibration method from [Vinel et al., 2021], residual distortions may remain introducing a bias in the DIC measurements. An estimation of potential biases hiding within the SIF , v_c and $T - stress$ identification showed discrepancies of $1MPa\sqrt{m}$, $0.1c_R$ and $3MPa$ respectively.

Remark 5.16. *From the experimental extraction on TAF1, the $T - stress$ remains positive, however, a negative $T - stress$ is obtained in the simulation, the difference might find its roots in the difference of the crack-tip speeds which makes the crack-tip 'see' different loading/unloading histories. It's mentioned that in the other samples (Appendices G, H and I) a negative $T - stress$ is estimated after the initiation.*

From here, we report the evolution of the direction of $\pm\theta_0$ at different positions of the crack-tip inside the simulation in Figure 5.20. $r_c = 2mm$ is also considered consistently with the previous experimental findings.

Observing the obtained trend of θ_0 , we see the following:

- the fracture direction is first along the crack growth;
- instabilities are predicted to occur earlier than in the experiment (a question arises here: can these instabilities relate to damage band widening before branching?)
- $\sigma_{\theta\theta}$ increases to around $70MPa$ and drops as the direction of propagation θ_0 becomes different than zero.

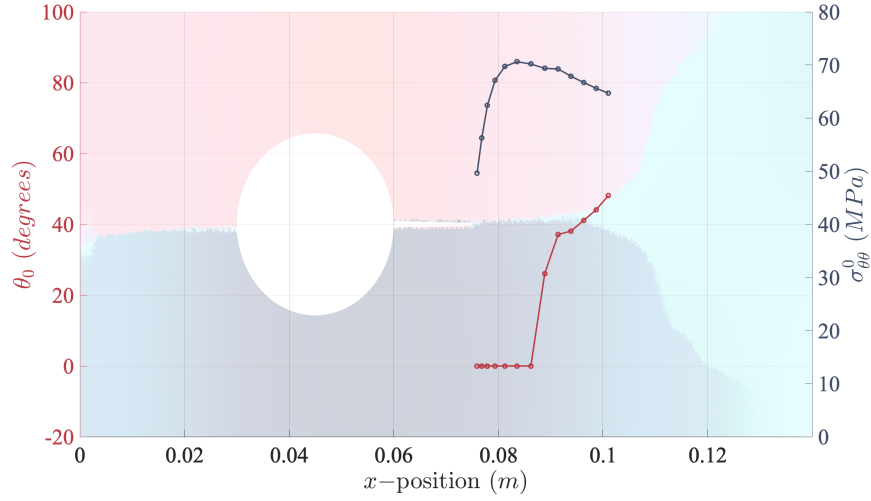


Figure 5.20 – Evolution of the predicted fracture direction θ_0 along with the maximum circumferential stress computed at $r_c = 2\text{mm}$ in the phase-field simulation of the TAF1 sample (SIF , T -stress and v_c from the numerical fields). The modification of the fracture angle θ_0 at the position of branching and the evolution of $\sigma_{\theta\theta}^0$ mirror the experimental branching.

Simulation results on the (in)stability map

By superposing the crack propagation history (v_c, T -stress) on the experimentally-built material instability map from Figure 5.15, we obtain the patterns in Figure 5.21.

Evidently, the history of crack propagation is much different than that in the experiments, even though it was accurately able to reproduce the crack patterns. The instability map shows the initiation of the propagation from the notch (circle marker) through the square marker corresponding to the damage band widening, until the moment of detection of branching (arrowhead). The map accurately shows a transition between the stable and unstable zones at the widening of the phase-field damage band: at negative T -stress but at a high tip speeds. Afterwards, as the damage continues its straight propagation and reaches the branching position, T -stress is closer to the experimental T -stress, but the crack-tip speed is always larger. The predicted stress (Figure 5.21) is larger in the phase-field simulation. We believe that a more robust identification of the phase-field parameters is required to enable a better reproduction of the experimental crack patterns, crack-tip speeds and eventually crack growth in the (v_c, T -stress) space.

Remark 5.17. We're not sure how/if phase-field's length scale l_c is linked to this r_c , more

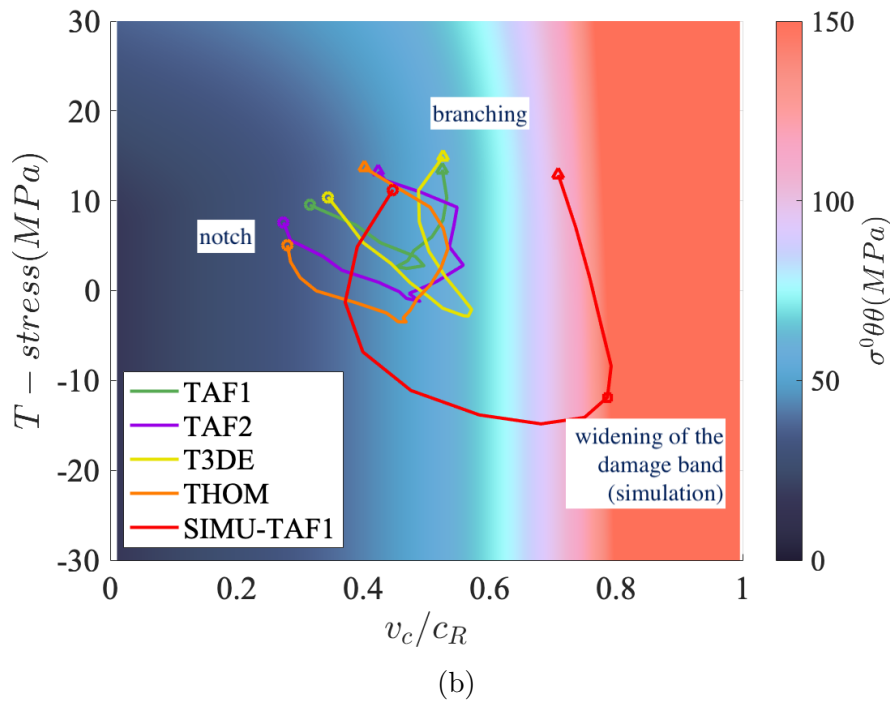
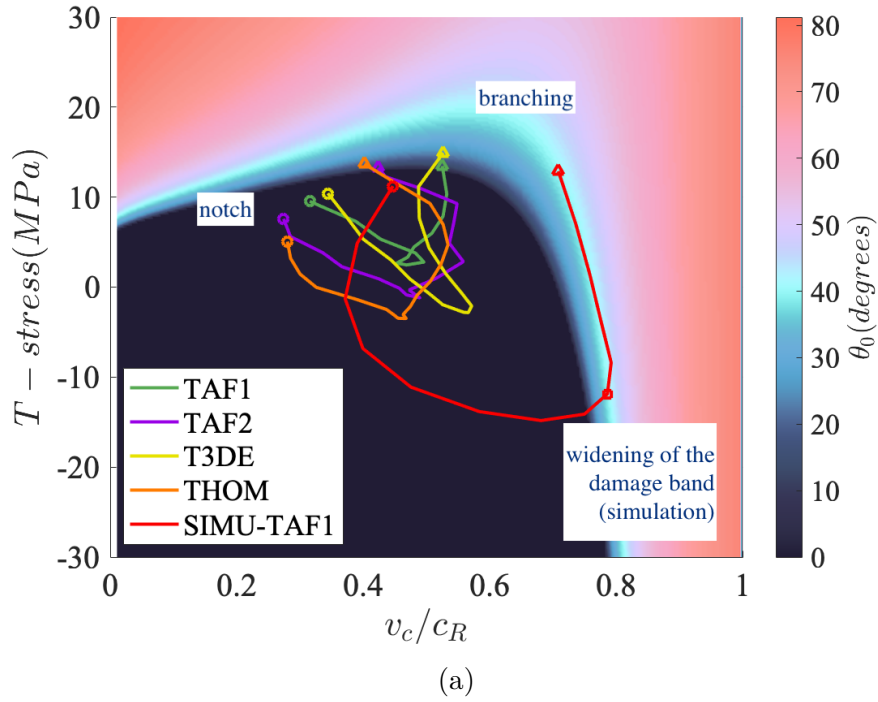


Figure 5.21 – (In)stability map of PMMA, constructed from experimental measurements and fitted to [Kanninen and Popelar, 1985]’s empiric law. The history of the crack propagation in each sample is displayed; from the initiation at the notch (circular marker) until the branching position (upward-pointing arrow) ± 1 frame, the map accurately predicts the (in)stability at the branching position with the change of θ_0

investigations should be lead to further elaborate on this point.

We summarise this application on the phase-field simulation by drawing the following points regarding:

- The phase-field model is able to accurately reproduce the crack patterns even in cases where the stress-waves play a major role on the crack propagation. However,
- UHS-HR imaging couples with the cutting-edge *DIC* algorithms allow a meticulous comparison of the crack propagation histories, and
- Unfortunately, the parameters herein used might not be the most accurate, as they are obtained by trial and error on the simulations to fit the pattern, the crack-tip speeds couldn’t be recovered.
- The proposed methodology to assess the (in)stabilities shows how the history of the crack growth, despite the accurate replication of the crack patterns, is not reproduced.
- Most prominently, the (in)stability map accurately predicts the crack branching and damage band thickening in the phase-field model as an interplay between the crack-tip speed and $T - stress$

After validating the applicability of the proposed criterion on a phase-field simulation, the next section wraps-up this final chapter by repeating the analysis on the benchmark proposed by [Borden et al., 2012]. This would further validate the robustness of the criterion thanks to the distinctive branching phenomenon in this benchmark.

5.8 Validation of the role of $T - stress$ on crack branching in [Borden et al., 2012]’s benchmark

After numerically advocating the dynamic crack instabilities on the phase-field simulation of the inertial impact test, we turn into an application of this analysis scheme on the benchmark [Borden et al., 2012].

Unlike the inertial impact test, in [Borden et al., 2012]’s benchmark there is:

- **no external loading along the direction of crack propagation is present** ,
- yet the crack branches at
- relatively low crack-tip speeds.

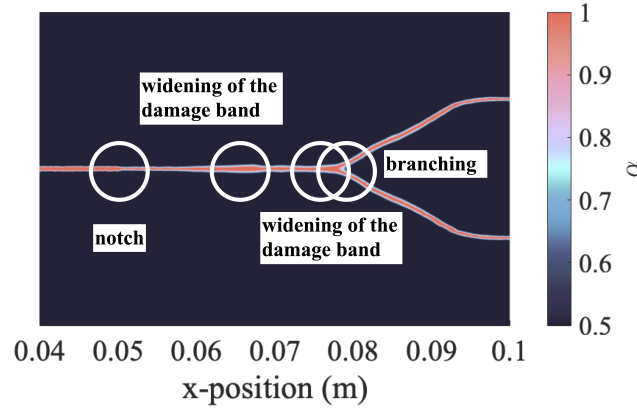


Figure 5.22 – Final damage state of the standard dynamic crack branching test [Borden et al., 2012], Appendix A, Chapter 1

And we aim to understand

- (i) Why does the crack not branch at its peak speed ($t \simeq 31\mu s$)?
- (ii) Why does it branch after, at lower speeds? and finally,
- (iii) What does the broadening of the phase-field at the branching position and beforehand actually mean?

And the answers to these questions of course are sought by applying the methodology to assess the instability source thoroughly discussed in the previous section.

As we'll see, the estimation of SIF , $T - stress$ and v_c would show an emergence of a positive $T - stress$. And the co-action of this $T - stress$ with the rapid running crack enables the methodology to successfully predict the (in)stability conditions and the branching angle. And more importantly, the (in)stability maps gives insights on the damage band thickening observed in the phase-field simulation.

Figure 5.22 shows the final damage state of the material.

5.8.1 On the crack path history

The description of the crack path history can be found in Section 1.9.2. We recall some of the main points:

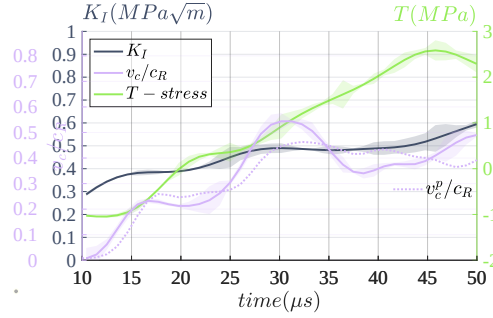


Figure 5.23 – SIF , the higher order term $T - stress$ and the crack-tip speed in [Borden et al., 2012]’s benchmark, the error-bar corresponds to the sensibility to the extraction zone. The crack-tip speed v_c^p corresponds to the one reported in Figure 5.18 computed from the phase-field, via Appendix B

- the crack is initiated after $t = 12\mu s$ of constant loading
- no branching occurs at its maximum speed ($t = 31\mu s$), only broadening of the damage band (until $t = 36\mu s$)
- the crack decelerates and two branches bifurcate at an angle $\theta_0 = \pm 25^\circ$ at $t = 48\mu s$

Regarding the damage band width:

- The damage band broadens from $t = 31\mu s$ to $t = 36\mu s$; the crack propagates stably
- The damage band broadens from $t = 43\mu s$ before branching at $t = 48\mu s$.

Remark 5.18. Also in this simulation, branching is preceded by a widening of the damage band.

To advocate these distinctive phenomena we apply the scheme of analysis proposed previously on the simulated displacement fields $\underline{u}_{sim}$.

The intermediate step requires the evaluation of SIF , $T - stress$ and the crack-tip speed from the application, its results are shown in Figure 5.23.

Instability prediction

From $x = 0.05m$ to the position of branching, both K_{ID} and $T - stress$ are increasing but the crack-tip speed is oscillating. A peak in the crack-tip velocity is found at $t = 31\mu s$. The errorbar shows inaccuracy of the extraction results (K_{ID} , $T - stress$, and crack-tip

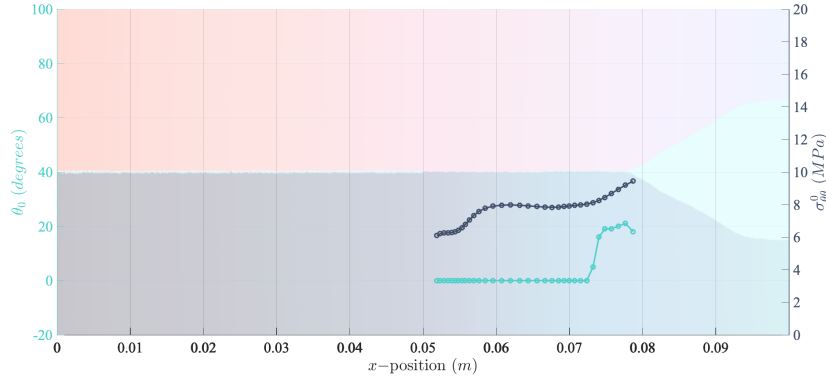


Figure 5.24 – Evolution of the predicted circumferential stress $\sigma_{\theta\theta}^0$ and the fracture direction θ_0 along the crack propagation of the benchmark in [Borden et al., 2012]

speed) after $t = 50\mu s$, suggesting thus that the branching may have occurred around this time step⁸.

Of course, the critical distance r_c should be determined next. Following previous developments, r_c is to be set as the value of r_o [Ramulu and Kobayashi, 1983] at the branching frame. Since the phase-field modelling does not explicitly represent the crack (regularisation of the discontinuity), the exact frame of branching cannot be accurately determined, this might lead to slightly inaccurate predictions of r_c .

In phase-field models, branching might be preceded by a widening of the damage band, this widening starts earlier (earlier than the time the branches are detected). The computation of the critical distance r_c for instabilities at the damage band broadening just before branching (Section 5.3) seems a reasonable speculation. This estimates r_c around $600\mu m$. This value yields accurate predictions of the branching angles.

Using this value of r_c , Figure 5.24 shows the fracture angle θ_0 and $\sigma_{\theta\theta}^0$ along the crack propagation from the notch to its branching position. For the crack-tip between $x = 0.05m$ and the position of branching, the predicted fracture direction from these data is obtained in the elongation of the crack, consistently with the simulation observation. The maximum $\sigma_{\theta\theta}^0$ stress in this region of propagation increases rapidly from $6MPa$ at $v_c = 0.23c_R$ to a plateau at $8MPa$ along the stable crack propagation before branching. $\sigma_{\theta\theta}$ increases as the direction of fracture θ_0 deviates from 0° to 25° at the branching position.

The arisen instability at this location (the increase in the maximum stress with a change in the fracture angle) induces the branching. Consistently, the measured branched

8. From the simulation's damage field, branching is found to occur at $t = 48\mu s$, after some widening of the damage band

angle from the simulation is equal to $\theta = 55^\circ \simeq 2\theta_0$. Branching occurs at a relatively low crack-tip speed ($v_c \simeq 0.4c_R$) in the presence of a positive $T - stress \simeq 1.3MPa$.

Once again, the direction of maximum circumferential stress computed at r_c from the crack-tip from the asymptotic solution successfully predicts the crack branching angle.

We then construct the material (in)stability map and superpose the history of the dynamic loading. To do so, we assume that the evolution of K_{IDC} follows Equation 5.7, K_{IC} and m are fitted on [Kanninen,]'s model from the extracted SIF along the dynamic crack propagation before the branching. We obtain:

$$\begin{aligned} K_{ID} &= 0.445MPa\sqrt{m} \\ m &= 3.2 \end{aligned} \tag{5.8}$$

The (in)stability map is given in Figure 5.25. The focus will be shed on the $(v_c, T - stress)$ space. The crack propagation history is superposed on the map. From the notch, the crack propagates at increasing v_c and $T - stress$. It heads towards the transition zone around $v_c = 0.54c_R$ and $T - stress = 1.07MPa$ at $t = 31\mu s$. This time corresponds to the beginning of crack widening observed in Figure 5.22. The propagation history then shows a decelerating crack that would enter the transitional zone at $v_c = 0.38c_R$ and $T - stress = 2.49MPa$, corresponding to $t = 43\mu s$, the time at which the damage band is observed to broaden just before its branching.

The (in)stability map also predicts that maximum stress would occur at the first widening of the damage band ($t = 31\mu s$). Once again, the maximum value of $\sigma_{\theta\theta}^0$ herein reached does not necessarily account for crack branching. Here, the closeness to the transition zone destabilises the crack and broadens the damage band but without inducing branching. Then as the crack propagation history curve enters the transitional zone, the damage band is observed to broadens before branching. Having $\theta_0 \neq 0$ is a sufficient condition for branching while having the stress surpass a certain threshold is only necessary.

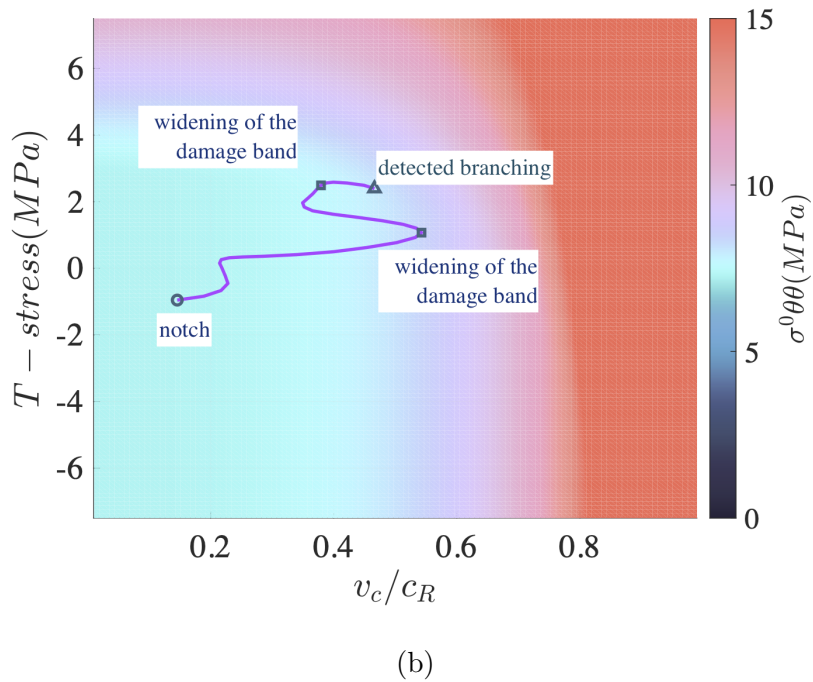
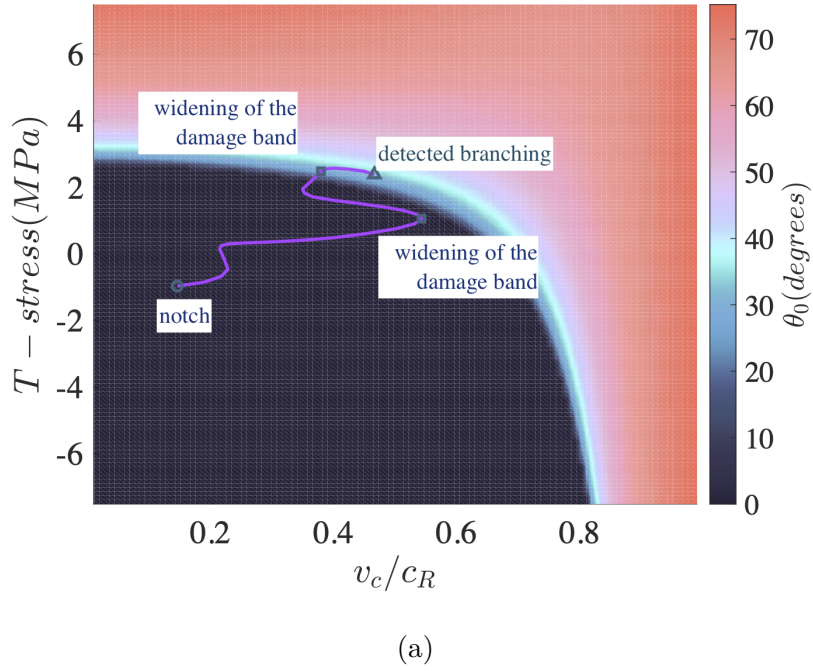


Figure 5.25 – (In)stability and maximum circumferential stress maps of the benchmark, constructed from [Borden et al., 2012]’s simulation results. The history of the propagation is shown in purple, the initiation from the notch (circular marker), the two widenings of the damage band (square markers), and the branching (upward-pointing arrow) are all reported on the maps

5.9 Concluding remarks

The unquestionable influence of the stress-waves on the crack propagation and their interactions with a moving crack-tip in a homogeneous material were highlighted in this final chapter. The analysis is lead in the *SIF* (dynamic fracture mechanics) concepts.

We combined UHS-HR imaging technologies with cutting edge *DIC* algorithms on a novel experimental inertial impact test. A distinctive geometry that would yield interesting crack propagation and branching phenomena is considered. This configuration allowed the measurement of never-seen-before $400kfps$ full-field kinematics. The most compelling captured phenomena are the compressive stress-waves entering the specimen, the cracks initiation and propagation, and of course crack branching as tensile stress-waves lengthwise of the crack meet its tip.

DIC measurements allowed the extraction of relevant information regarding the fracture process, knowingly *SIF*, $T - stress$ and the crack-tip speeds. From here, we showcase the role played by $T - stress$ on the crack branching phenomena by analysing the direction of maximum circumferential stress at a reference distance r_c from the crack-tip along the propagation. Indeed instabilities are fostered as a co-action between the rapid propagating crack and the presence of a stress lengthwise of the crack direction $T - stress$.

Afterwards, we build a comprehensive (in)stability map that enables the assessment of the unquestionable role held by $T - stress$ on crack branching and instabilities at relatively low crack-tip speeds. Indeed, this criterion predicted crack instabilities at lower crack-tip speeds than elaborated in the classical dynamic fracture theory. A validation of the analysis scheme is also lead on crack-branching phase-field simulations.

The most compelling findings are summarised as follows:

- (i) $T - stress$ plays a major role in dynamic (in)stabilities and limiting crack velocities. This role is put forth both experimentally (highly resolved ultra-high-speed imaging + *DIC*) and numerically (phase-field simulations).
- (ii) The (in)stability map constitutes a straightforward visual tool for assessing dynamic (in)stabilities based on simple fracture mechanics concepts. The modification of the angular distribution of the stresses at a distance from the crack-tip due to its speed and the presence of $T - stress$ are at its core.
- (iii) A phase-field simulation of the inertial impact test, although accurately predicts the crack patterns, fails in exactly reproducing the crack-tip speeds and crack history. Despite that, the superposition on the experimental (in)stability map accurately

predicts the branching phenomenon, and illustrates how the underlying mechanisms (experiment versus its simulation) are fundamentally different.

- (iv) Before branching, damage bands are observed to widen. From the instability map, we see how the widening coincides well with a deviation into the transition zone (between stable and unstable crack propagation)
- (v) After validating the capability of the proposed method to predict branching in phase-field simulation results, we went back to a crack branching benchmark in which no loading along the crack propagation exist, and hence intuitively no $T - stress$ should appear. Surprisingly, the observed branching develops as a positive $T - stress$ appears at the crack-tip.
- (vi) Further, the (in)stability map of the benchmark shows how damage bands widening can also be explained via the proposed analysis scheme by noticing tilting into the unstable zone.

We believe that the insights given here on the crack-branching as a result of the interplay between a moving crack-tip v_c and $T - stress$ in homogenous materials, should build the foundation for future prospectives regarding numerical simulations and investigations of dynamic failure in more complex materials.

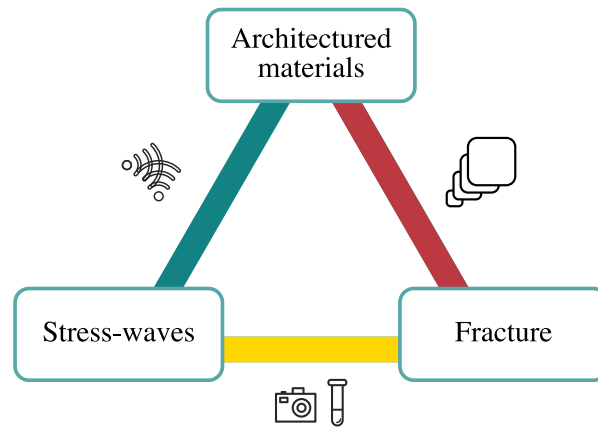
PART IV

Conclusion and perspectives

CONCLUSION

This study sets up the foundations for the multi-scale analysis of dynamic fracture in architected materials. We aimed at analysing the interaction between architected materials, stress-wave and crack propagation, through analysis on three model architected materials.

We broke-down the problem into three sub-problems **Eventually, bringing forth the necessary tools towards a multi-scale analysis of dynamic fracture of architected materials.**



After providing the necessary theoretical background relevant to brittle fracture, architected materials, numerical simulations and homogenisation techniques, we first presented the phase-field model that was used for the micromechanical simulations. An extension was proposed via a parametrisation of the elastic strain threshold. We showed how this contribution enabled the phase-field model even more versatility without adding to its complexity. It allowed the decoupling of the regularisation scale, the strength and the toughness of the material model. Application and validation of the influence of this parametrisation on the material response in a quasi-statics and in a dynamics benchmark

validate the applicability of this extension within the consistent framework.

Secondly, we proposed a versatile model-free coarse-graining approach that is indeed applicable on cases where the statistical homogeneity of the material ceases to exist (Quasi-Periodic materials with long-range heterogeneities) and more importantly when sharp localisations are present. The method bridged the brittle behaviour at the microscopic scale to the quasi-brittle behaviour at the mesoscopic scale. The notion of strength and toughness naturally emerges. This method validates the use of the quasi-brittle models and suggests non-locality of the softening process.

Next, we debuted the multi-scale analysis of dynamic fracture of architected materials by analysing the crack propagation inside architected materials at multiple scales. We started by simulating the failure process of architected materials at the microscopic scale via the phase-field model and followed by coarse-graining the obtained micromechanical fields to mesoscale fields.

- ▶ We've seen how the crack tends to follow the path that would allow it maximum energy dissipation, it's found that the crack avoids 'resilient patterns' in the Quasi-Periodic material and follows 'weak' planes in the Periodic material.
- ▶ The effective fields of mechanical properties are established at different coarse-graining scales, from here, and without any a priori on the material's behaviour, a genuine evaluation of the effective material and failure properties was provided (density, elasticity, strength, toughness and effective crack path).
- ▶ By definition, the mean density is conserved across the scales.
- ▶ We show that in order to consider a homogeneous isotropic elastic equivalent medium, the required length scale exceeds the values considered in the literature and in fact is much larger when considering non-periodic microstructures with long-range heterogeneities.
- ▶ The fracture strength computed as the critical stress along the crack propagation is found to be the hardest to smear-out; in fact, the influence of the microstructure persists in all three microstructures even for relatively large coarse-graining scales.
- ▶ Coarse-graining shows good ability to smear-out the microstructural effects on the effective toughness.

This analysis lead us to believe in the inevitability of the consideration of a **non-homogeneous** material in which the influence of substructures is preserved at the mesoscopic scales. Moreover, the discrepancy between the 'homogeneity' of the failure properties

dismantles the unique relation relating the fracture toughness, the length scale and the strength.

We continued the analysis by tackling the damping of stress-waves inside architected materials; we did so through analysing finite element simulations of transient wave-packet propagation. The kinetic energy attenuation performance was compared between the three microstructures.

Further, we shed light on the wavelengths components of the wave-packet exiting the considered microstructures. The periodicity of the microstructure and the wavelengths of the stress-waves play a major role on the propagation and/or scattering of the stress waves.

- For different wavelengths, the energy localisation inside the architected materials shows different patterns, in the Quasi-Periodic materials 1, the resilient patterns normally avoided by the crack path are also avoided by the stress-waves.
- The effective attenuation/damping/dissipation of energy actually results from waves spreading due to scattering inside the architecture at the free boundaries and the amazing capabilities of the Quasi-Periodic microstructure to damp the stress-waves is noted (probably due to the long-range pattern heterogeneities in the Quasi-Periodic microstructures providing continuous source of scattering).
- Bandgaps are shown to exist in the three microstructures, with an increase in the Quasi-Periodic microstructures, a signature of their long-range heterogeneities in their patterns.

The superiority of the Quasi-Periodic is once again advanced regarding its overall better dynamic properties (stress-wave scattering, attenuation, bandgaps, etc.) as compared to the Periodic one.

Finally, we analysed the role of stress-waves on the crack propagation and their interactions with a moving crack tip in a homogeneous material, as a first step towards the dynamic analysis on architected materials.

For this sub-problem, We combined UHS-HR imaging with cutting edge *DIC* algorithms on a novel experimental inertial impact test on a distinctive geometry. We followed the stress-waves and crack propagation inside the material. The analysis is lead in the stress intensity (dynamic fracture mechanics) concepts, based on the maximum circumferential stress.

We built a comprehensive (in)stability criterion that enables the assessment of the unquestionable role held by $T - stress$ on crack branching and instabilities at relatively

low crack tip speeds. Validation of the analysis scheme was also lead on crack-branching phase-field simulations.

- ▶ As stress-waves are reflected back and forth from the free boundaries, the crack tip is loaded and unloaded alternatively.
- ▶ By introducing a length scale, we analyse the role played by $T - stress$ on crack instabilities, and
- ▶ We experimentally built a comprehensive (in)stability map that separates the stable from the unstable crack growth as a function of the couple $(v_c, T - stress)$.
- ▶ Indeed, this map was able to explain the crack branching at lower crack tip speeds than elaborated in the classical theory.
- ▶ A phase-field simulation of the inertial impact test, although accurately predicts the crack patterns, fails in exactly reproducing the crack tip speeds and crack history. Despite that, the superposition on the experimental (in)stability map accurately predicts the branching phenomenon, and illustrates how the underlying mechanisms (experiment versus its simulation) are fundamentally different.
- ▶ Before branching, damage bands are observed to widen. From the instability map, we saw how the widening coincides well with a deviation into the transition zone (between stable and unstable crack propagation).
- ▶ After validating the capability of the proposed method to predict branching in phase-field simulation results, we went back to a crack branching problem in which no loading along the crack propagation direction exists, and hence intuitively no $T - stress$ should appear. Surprisingly, the observed branching develops as the co-action of a positive $T - stress$ at moving crack tip speed.
- ▶ Further, the (in)stability map of the benchmark shows how damage bands widening can also be explained via the proposed analysis scheme by noticing tilting into the unstable zone.

We believe that the insights given here on the crack-branching as a result of the interplay between a moving crack tip v_c and a $T - stress$ in homogenous materials, should build the foundation for future prospectives regarding numerical simulations and investigations of dynamic failure.

PERPSECTIVES

The present thesis has explored the vast field of the multiscale dynamic failure in architected materials with a special attention on a set of Periodic and Quasi-Periodic lattices of holes. It also tackled the branching phenomenon in homogeneous materials.

Yet, there are many potential research directions from the results and methodologies developed in this work, and some questions remain to be answered.

Future work could be perused in the same spirit for applications on the dynamic failure of architected materials. This should further validate our most recent simulations regarding an inertial impact test on architected materials (Figure 5.26), where it's clear how the lattices of holes impact the dynamic crack propagation, similarly to the static crack propagation.

Also, coarse-graining of the field can yield a continuum description of the dynamic failure of such materials. And a multi-scale analysis of the branching can then be achieved. One might expect the small branches emerging at the microscopic scale to translate to damage band thickening or actual branching at the mesoscopic scales (Figure 5.26). Constructing coarse-grained (in)stability maps might give insights on the influence of the coarse-graining on the branching response, and elaborates on the role of the heterogeneities in increasing the critical distance r_c making the cracks more prone to branching.

The experimental work initiated in this thesis didn't get the importance it deserved in the manuscript, since we only exploited it as a tool not as a purpose.

We mention that in the inertial impact test, the impact wave's width is related to the size of the projectile and the waveguide, hence the wavelengths in-play are much bigger than the microstructure's lengths, so attenuation of the stress-waves from the scattering (following Chapter 4) is improbable. From here, finding a configuration in which stress-wave damping plays a major role in reducing the energy available in the vicinity of a crack and hence modifying its growth behaviour is essential. This should lead to further exposure on the performances of the architected materials.

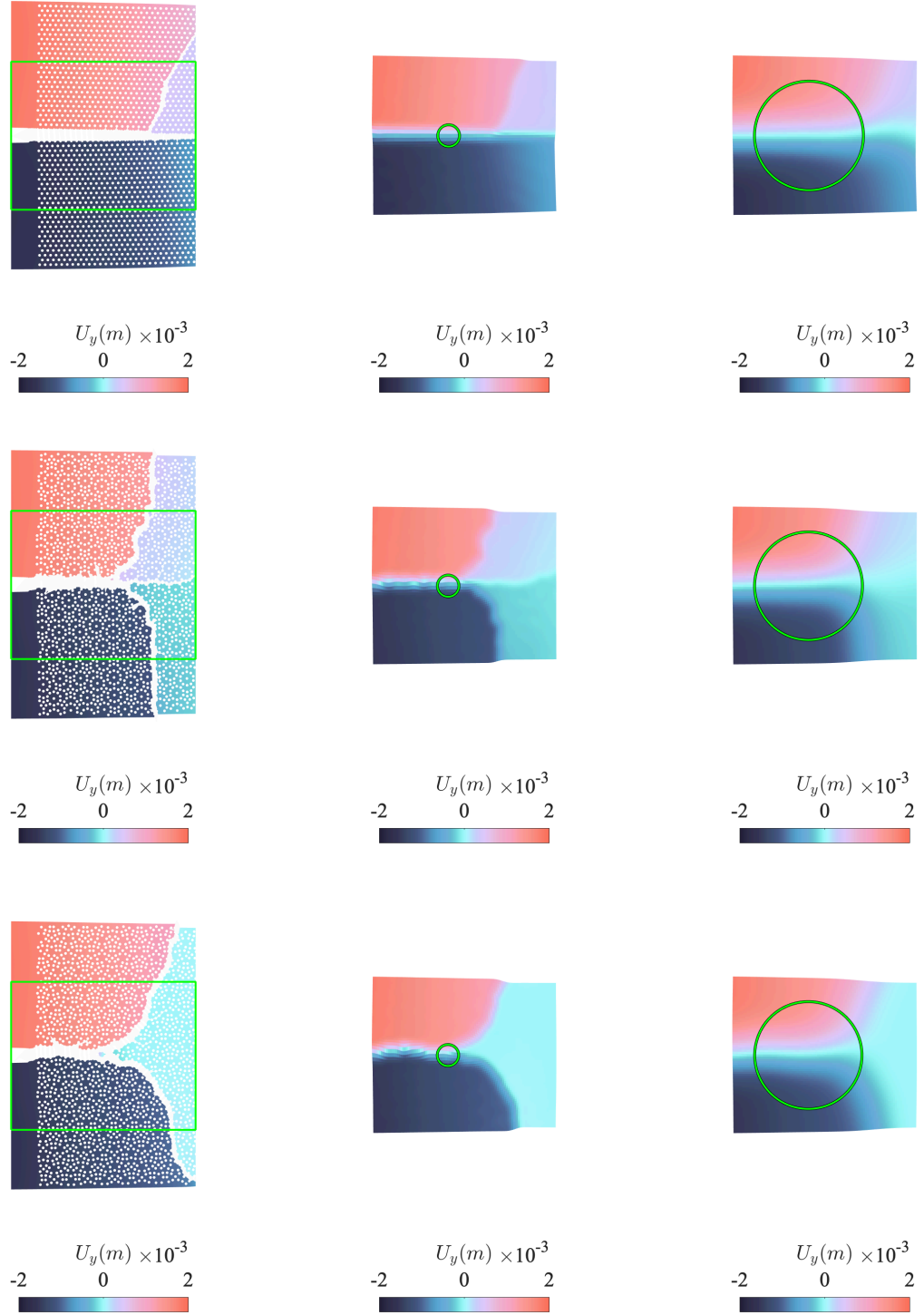


Figure 5.26 – Inertial impact test simulations of the Periodic (up), Quasi-Periodic type 1 (middle) and Quasi-Periodic type 2 (down) materials. Coarse-grained displacement fields at $l_{CG} = 2d$ and $10d$ are shown (l_{CG} is the radius of the dark green circles, they're computed on the coarse-graining support domain (green rectangle))

From *DIC* algorithms, coupled with UHS-HR imaging, one can propose a sound strategy that would allow a more rigorous identification of the phase-field parameters based on a coupling between the crack tip speed, extractions of *SIF* and higher order terms. With the extension proposed to the phase-field model, more freedom is granted on the choice of phase-field parameters, and we believe that an application similar to the one where the crack tip positions are directly confronted with the simulations' (inspired from [Réthoré and Estevez, 2013]) should help the phase-field modelling community in their quest in accurately simulating failure without adding to the complexity of the problem.

Even though the phase-field modelling is a robust approach that requires no artificial criteria for crack initiation, crack coalescence or crack branching, the resolution is usually made over the whole domain which naturally makes simulations computationally heavy. From the material (in)stability a simple criterion for crack branching naturally emerges. We expect computationally efficient methods like X-FEM [Moes et al., 1999] to be enriched with such an effective criterion to judge crack branching. Instead of the more costly methodologies, knowingly the ones based on enriching the classical displacement field to model a multiple branched crack (via 'junction' functions [Daux et al., 2000] to relate two or more cracks), or the ones based on the loss of hyperbolicity [Belytschko et al., 2003], we believe that the herein proposed criterion can be a lighter alternative to study the branched crack using X-FEM. Evaluating $T - stress$ via an interaction integral method for example ([Paulino and Kim, 2004]) is a relatively straightforward task, and by carefully incorporating the critical distance r_c , the (in)stability map enables an effortless analysis of the (in)stabilities and crack branching.

Can r_c be linked to the notion of a process zone? We believe that r_c , as a critical distance that explains phenomena near the crack tip that couldn't be explained from fracture mechanics otherwise, is a philosophically sound concept to be related to the notion of a process zone. In PMMA, in stress-controlled static brittle fracture of PMMA the process zone size has been suggested to be $0.5mm$ [Chao and Zhang, 1997]. Much smaller than what we found in our analysis. We believe that linking these two quantities is an interesting avenue to be explored.

PART V

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PART VI

Appendices

DYNAMIC CRACK BRANCHING: THE INFLUENCE OF THE PHASE-FIELD PARAMETERS

Further examples showcasing the influence of the phase-field parameters on the crack paths and crack tip speeds for the benchmark proposed by [Borden et al., 2012] are showcased in this appendix.

After we've seen the influence of the elastic threshold $\phi_{c,c}$ on the outcome of the phase-field simulation, we showcase examples demonstrating the effect of the length scale parameter l_c and the fracture toughness g_c . Moreover, we fix the resistance (or critical stress) σ_c (via Equation 1.52) and analyse the phase-field simulation results. All cases will be compared to the standard result, i.e., [Borden et al., 2012] with the benchmark's parameters: $E = 32GPa$, $\nu = 0.2$, $l_c = 0.25mm$, $g_c = 3J/m^2$ and no threshold. Plane strain conditions are assumed.

When varying a parameter, the others are fixed to the benchmark's. For each investigated parameter, two values are considered and the results are compared to the benchmark's. The three crack paths are showcased side-by-side; [Borden et al., 2012]'s result are put on the left. The crack tip speeds are then superposed on the same plot. The dark plots correspond to the main crack, blue (and green when available) represent the branches in the lower half of the sample.

A.1 Influence of g_c

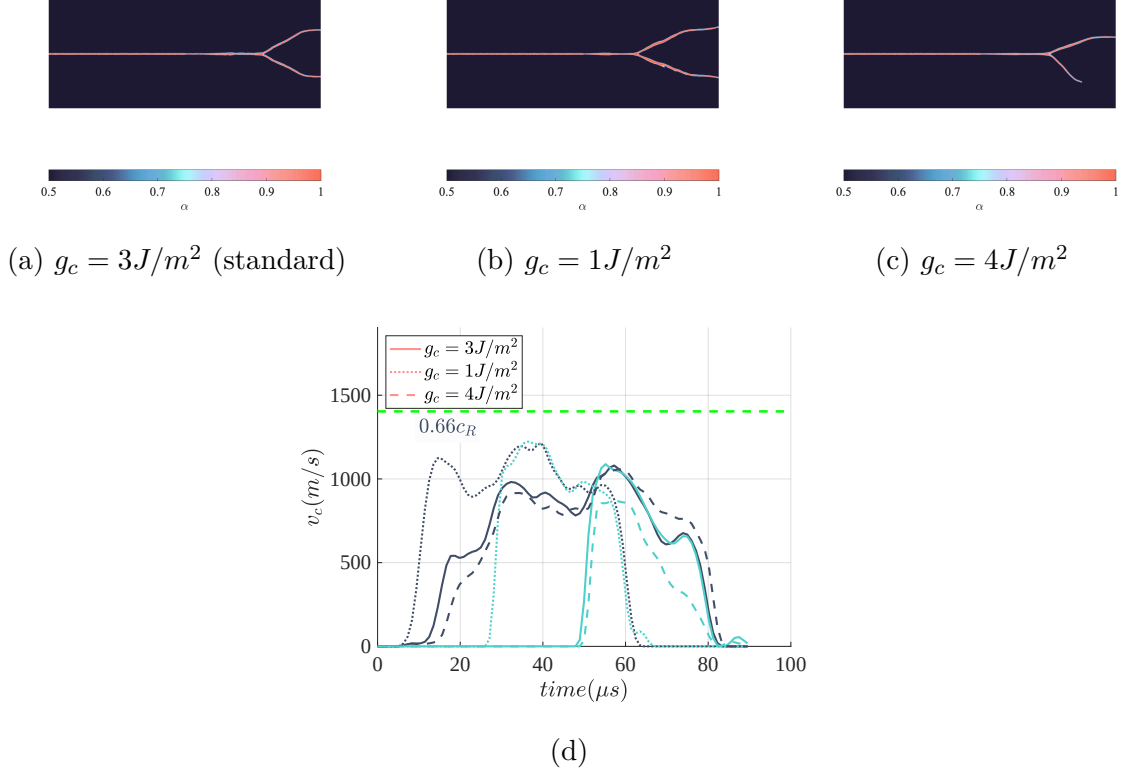


Figure A.1 – Fracture patterns and crack tip speeds for different g_c , comparison with the work of [Borden et al., 2012] (a)

Results of three g_c are displayed with $l_c = 0.25mm$ and no elastic threshold. For a smaller $g_c = 1J/m^2$ (Figure A.1(b)), the two branches are longer than the branches in the standard $g_c = 3J/m^2$ (Figure A.1(a)). For $g_c = 4J/m^2$, the branches are no more identical nor symmetrical (Figure A.1(c)). Figure A.1(d) shows the crack tip speeds for the three cases. The crack at $g_c = 1J/m^2$ is initiated in advance as compared to the standard one, and is systematically faster and reaches a higher maximum speed. At smaller g_c , the creation of new surfaces from the available energy is easier and faster [Broberg, 1996, Broberg, 1964]. The crack also branches earlier ($-20\mu s$). The two branches propagate at similar speeds. At $g_c = 4J/m^2$, the crack initiation is delayed of about $5\mu s$ as compared to the standard $g_c = 3J/m^2$. The speeds are slightly slower. The bigger g_c translates to a slower damaging of the material, i.e., the creation of new crack surface require more energy [Broberg, 1996, Broberg, 1964] that should subsequently be available (from the

boundaries). The branches are no longer travelling at similar tip speeds and their symmetry is lost.

A.2 Influence of l_c

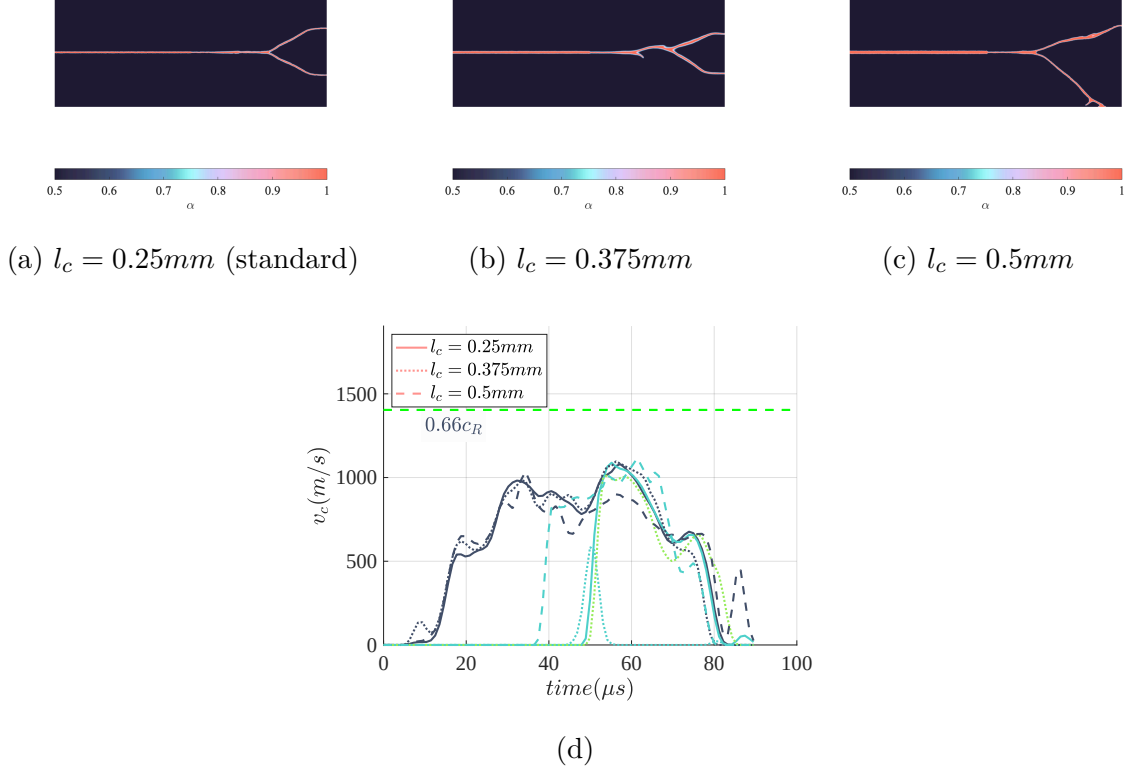


Figure A.2 – Fracture patterns and crack tip speeds for different l_c , comparison with the work of [Borden et al., 2012] (a)

Results of three l_c are displayed with $g_c = 3J/m^2$ and no elastic threshold. To overcome mesh-related bias, only two bigger l_c are considered. At $l_c = 0.375mm$ (Figure A.2(b)), the crack branches twice; however, its first branch is directly arrested, afterwards, even though the main crack is no longer along the middle of the sample, the symmetry of the two branches after the second branching are recovered. At larger $l_c = 0.5mm$ (Figure A.2(c)), the crack branches after travelling a shorter distance but the two branches are not symmetrical. One of the branches also undergoes a late branching phenomenon. The speeds at which the cracks travel in the three cases have similar trends. For $l_c = 0.25$ and $0.375mm$, the branching occurs at similar times and positions. For the largest $l_c = 0.5mm$, the earlier branching ($-10\mu s$) slows down the branches that would travel afterwards unsymmetrically and at different speeds.

A.3 Fixing σ_c

A.3.1 Fixing the ratio $\frac{g_c}{l_c}$

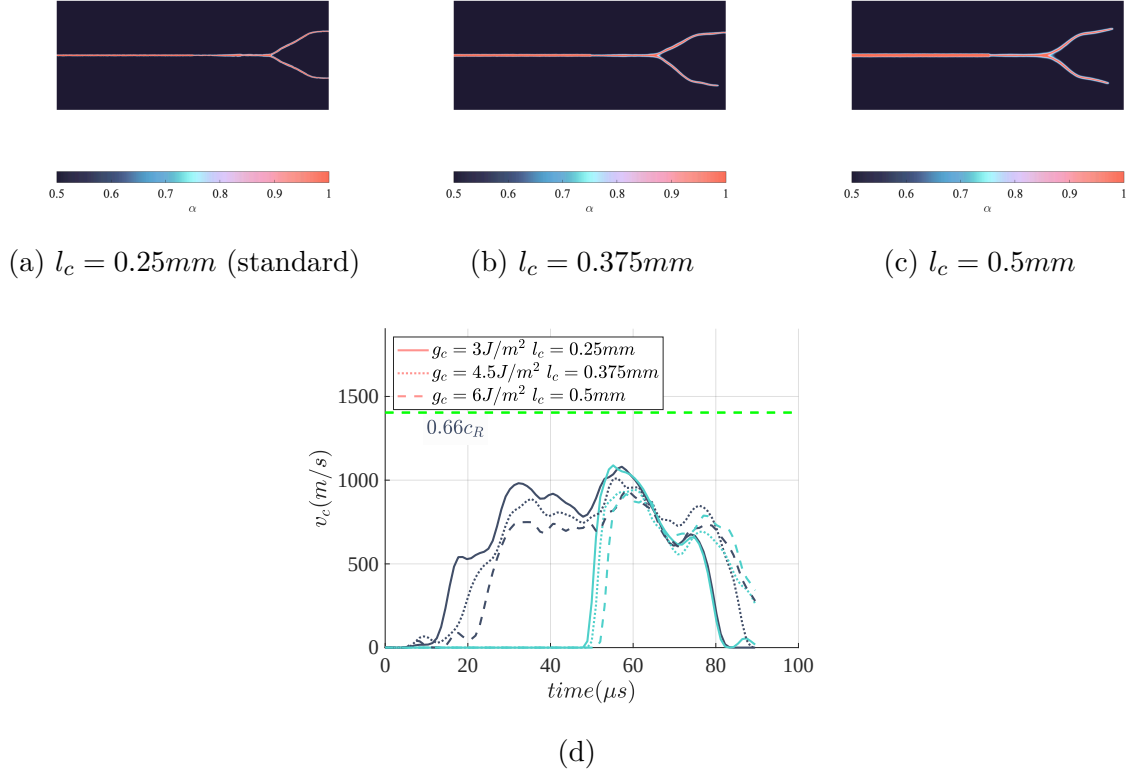


Figure A.3 – Fracture patterns and crack tip speeds for different (l_c, g_c) couples yielding same σ_c as [Borden et al., 2012] (fixed g_c/l_c), comparison with the work of [Borden et al., 2012] (a)

In Section 1.7, an expression of the critical stress σ_c was derived on a unidimensional bar under uniaxial tension; the expression states that a fixed ratio $\frac{g_c}{l_c}$ yields the same σ_c . Although this derivation is computed for a homogeneous unidimensional solution, following [Nguyen et al., 2016] we consider the derived expression to be a faithful estimation of the relation linking σ_c , l_c and g_c . We check the influence of fixing σ_c in the absence of a threshold by conserving the ratio $\frac{g_c}{l_c}$ on the benchmark results.

Results of three l_c are displayed with $\frac{g_c}{l_c}$ fixed and no elastic threshold. Previous results (Section A.1 and A.2) show similar crack tip velocities for different l_c and a big differences in velocities for different g_c in all cases, the crack patterns are different.

When increasing g_c and fixing the $\frac{g_c}{l_c}$ ratio, (Figure A.3(b), A.3(c)), the three simulations yield fundamentally similar crack patterns. At the smallest g_c , both crack branches reach the left boundary. The corresponding crack tip speeds are shown in Figure A.3(d). Larger g_c tend to delay the crack initiation and the branching, while maintaining fairly lower crack tip speeds. The maximum reached crack speed is also smaller at bigger g_c . The higher speeds after $t = 70\mu s$ are supposedly due to the fact that the branches are still propagating at the largest g_c and did not reach the right boundary yet.

A.3.2 Manipulating $\phi_{c,c}$ and l_c

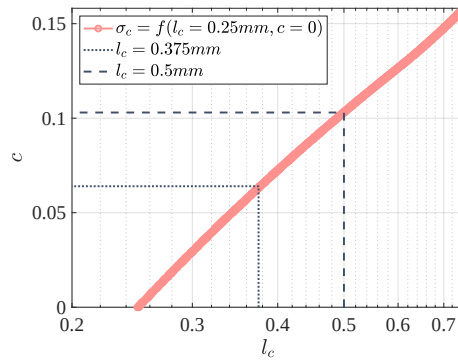


Figure A.4 – (l_c, c) couples yielding equivalent σ_c . Unidimensional solution from Equation 1.52, Section 1.8

In Section 1.8, an expression of the critical stress σ_c was derived on a unidimensional bar under uniaxial tension as a function of the threshold coefficient c , l_c and g_c . We check the influence of fixing σ_c (Figure A.4) by manipulating l_c and $\phi_{c,c}$, thus by eliminating the influence of g_c ¹. To do so, two couples of $l_c, \phi_{c,c}$ that yield similar σ_c at fixed g_c are obtained from Figure A.4. And simulations at fixed σ_c for three couples l_c, c are run. Surprisingly, the three crack paths (Figure A.5(a), A.5(b) and A.5(c)) are relatively similar. Moreover, Figure A.5(d) shows that the cracks branch in the three cases have identical histories, i.e., initiation and branching at close times, reaching similar maximum speeds, same deceleration and acceleration.

The influence of the different parameters of the phase-field model is showcased in this appendix. The additional freedom granted by the parametrisation of the elastic threshold

1. The influence of g_c was shown to be most prominent in Section A.1 and A.2, especially on crack tip speeds, as compared to the influence of l_c

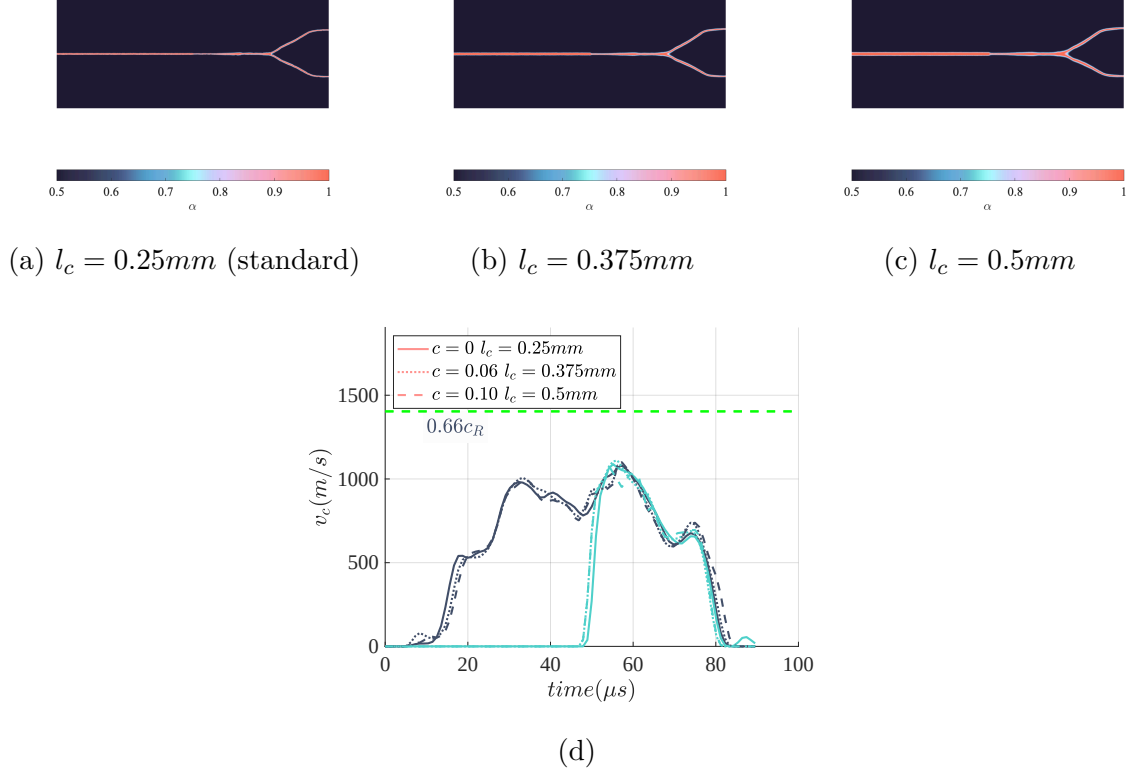


Figure A.5 – Fracture patterns and crack tip speeds for different (l_c, c) couples yielding same σ_c as [Borden et al., 2012], from Figure A.4, comparison with the work of [Borden et al., 2012] (a)

is seen as a promising addition to the phase-field modelling. It allows the phase-field even more adaptability for advanced simulations without adding to its implementation complexity. With the ability to consider a larger l_c for the simulations without affecting the critical stress σ_c or the toughness g_c , i.e., by manipulating the elastic threshold $\phi_{c,c}$, computational times can be improved.

CRACK PATH DETECTION

In this appendix an algorithm that allows for the automatic detection of multiple cracks is presented. In phase-field models (and any other continuous approach that does not explicitly represent the crack) determining the crack tips is not straightforward; since the crack is represented by a damage band of finite width related to l_c . This leads to inaccurate predictions of the crack tips translated to inaccurate predictions of the velocity for dynamic fracture [Wu et al., 2020]. With that in mind, we developed this algorithm to *automatically* detect crack *initiation*, *propagation*, and *branching* independently of the direction of propagation, number of cracks and crack arrest phenomena. Although crack coalescence is an interesting and widely encountered phenomenon, its detection was not implemented here. The algorithm requires the damage fields α at different time steps (loading steps) and the mesh data. It can be summarised by the following steps:

Crack tip detection from phase-field simulation results

For each time step t^n

- Find the newly damaged points $p_\alpha^n / \alpha(p^{n-1}) \leq 0.99 \ \& \ \alpha(p^n) \geq 0.99$
 - Regroup the newly damaged points p_α^n into i clusters c_i^n of maximum width $4l_c$ (see Remark B.2)
 - Compute the distance between each cluster
 - Combine clusters within a distance $2l_c$ into one cluster (see Remark B.1)
 - Determine the number of *unique* clusters N_c^n corresponding to actual crack tips c^n
 - If $\dot{N}_c^n < 0$, find arrested crack tips. $c_{i=a}^n = c_{i=a}^{n-1}$. Update N_c^n . Repeat. (see Remark B.3)
-

Here, at each time step t^n , N_c^n random crack tips c_i^n corresponding to the newly damaged points are detected, α is the damage phase-field (Chapter 1) representing the damage state of the material. ($\alpha = 0$ when intact, $\alpha = 1$ for a full damaged material, and $0 \leq \alpha < 1$ in the degraded zone.)

Next, the crack tips (across different time steps t^n) forming a single crack branch are combined. The history of each crack is thus computed from the position of its corresponding crack tips across the propagation.

For each time step t^n , under the condition $\dot{N}_c^n < 0$ For each crack tip c_i^n ,

- Compute the distance between c_i^n and each new cluster $c_{i=1 \dots N_c^{n+1}}^{n+1}$
- Obtain crack propagation history for each crack i

Remark B.1. *The chosen distance, here $2l_c$ of course conditions the branching detection, e.g., for a distance under $2l_c$, the crack tips are merged.*

Remark B.2. *The distances conditioning crack branching (here $2l_c$) and crack propagation (here l_c) can be modified per the simulation's requirements, i.e., if relatively large time steps are analysed (cracks advance by jumps), less conservative condition on crack arrest/initiation should apply.*

Remark B.3. *If the number of new c_i^n damaged points decreases (if $\dot{N}_c^n < 0$), this may suggest a crack arrest. The cluster corresponding to an arrested crack $c_{i=a}^n$ is conserved at*

upcoming iterations $c_{i=a}^{n+1} = c_{i=a}^n$. A tip is considered arrested if no new crack tips appear in its vicinity, i.e., the distance between $c_{i=a}^{n-1}$ and the closest $c_{i=1\dots N_c}^n$ is larger than l_c

ON THE PRESENCE OF A UNIQUE DAMAGE LAW

As the quasi-brittle behaviour of the effective material is set - independently of l_{CG} , an attempt to write a damage evolution law based on the coarse-grained stress-strain results (Figure 2.9) and the standard degradation function $g(\alpha) = (1 - \alpha)^2$ found in Chapter 1 was made. However it only worked-out under pure mode I loading. Of course, more work is required on this part to be able to link the two pillars of crack propagation: damage mechanics and fracture mechanics.

We follow the work of [François, 2012] by describing damage as a decay of the Kelvin moduli of the elasticity tensor. For a 3D isotropic material, the Kelvin decomposition yields two isotropic subspaces: a unidimensional hydrostatic one and a 5-dimensional deviatoric one. 6 Kelvin moduli exist (1 hydrostatic and 5 deviatoric). In 2D, only 3 Kelvin moduli exist $\lambda_I = \mathbf{K}$, $\lambda_{II} = \mu$, $\lambda_{III} = \mu$. $\mathbf{K}$ is the bulk modulus, μ is the shear modulus. (1 hydrostatic and 2 deviatoric).

Thanks to the symmetry properties of the mechanical fields at the vicinity of a pure mode I propagating crack, and due the regularizing nature of the coarse-graining, it's found that the deviatoric parts of the stresses and strains are omitted, and damage can only be observed in the hydrostatic subspace, and the degradation function will link the hydrostatic coarse-grained stress to the hydrostatic coarse-grained strain via

$$S_h = g(\alpha) \mathbf{K} E_h = (1 - \alpha)^2 \mathbf{K} E_h \quad (\text{C.1})$$

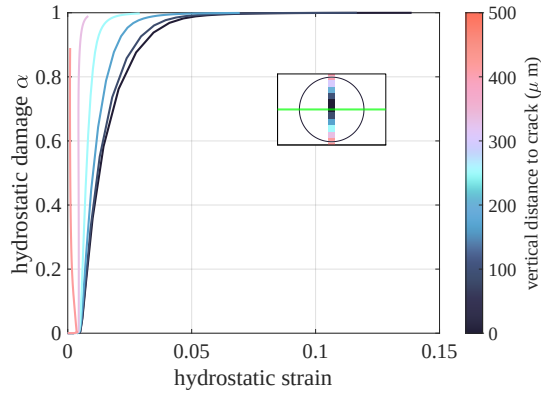
where S_h and E_h correspond to the hydrostatic parts of the coarse-grained stresses and strains respectively, and $\mathbf{K}$ is the bulk modulus of the sound material. α is the damage.

Figures C.1(a) and C.1(c) show the evolution of the damage α in the vicinity of the crack at two length scales l_{CG} . As seen, the non-uniqueness of the damage behaviour persists.

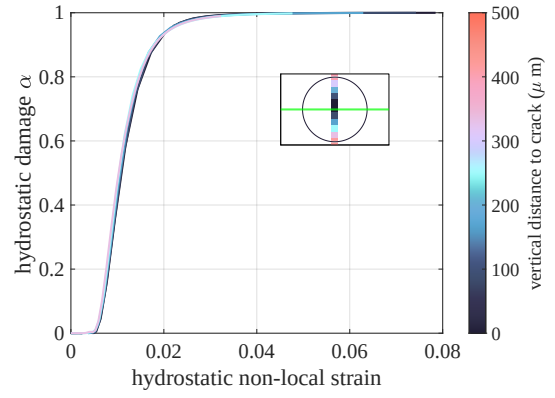
We were able to experiment with a non-localisation of the strains ($\tilde{E}_h = \langle E_h \rangle_{\phi_{l_{NL}}}$, a convolution with a regular function $\phi_{l_{NL}}$ of support l_{NL} ¹) to find a unique law relating the damage evolution to the non-local strains. In Figures C.1(b) and C.1(d), the non-local strains are computed within a non-local zone of size l_{NL} , and a unique damage evolution curve is obtained for the different points in the vicinity of the crack.

Even though a unique damage evolution law is obtained, its extension to combined mode *I* and *II* or with the addition of higher order terms, i.e., *T-stress* is more complicated. Future prospects require building on these intriguing findings to further advance on linking damage mechanics to fracture mechanics.

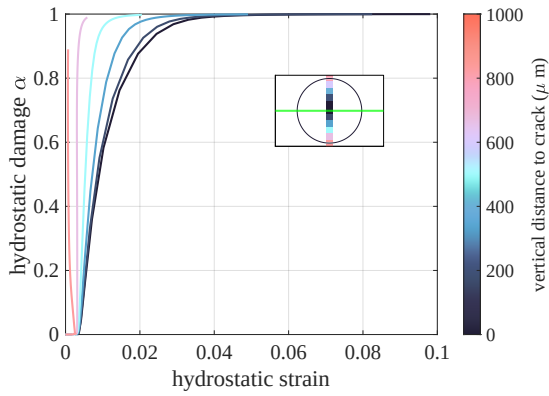
1. l_{NL} is to be related to l_{CG} . Based on our work, $l_{NL} \simeq 1.5l_{CG}$ is a fair estimation of the size of the non-local zone yielding a unique non-local damage evolution law.



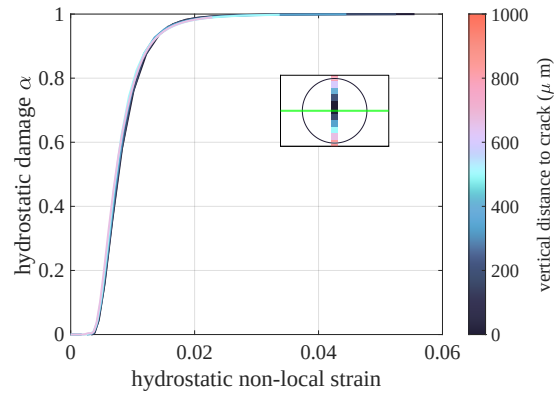
(a) $l_{CG} = 500\mu m$



(b) $l_{CG} = 500\mu m, l_{NL} = 1.5l_{CG}$



(c) $l_{CG} = 1000\mu m$



(d) $l_{CG} = 1000\mu m, l_{NL} = 1.5l_{CG}$

Figure C.1 – Coarse-grained hydrostatic damage evolution along the vertical direction at two length scales l_{CG} , non-localisation of the strains via a convolution with a regular function of support width $l_{NL} = 1.5l_{CG}$

STRESS INTENSITY FACTORS EXTRACTION FROM DISPLACEMENT FIELDS

D.1 *SIF* Theoretical aspect

The *SIF* and *T – stress* measurement is essential for validating the role of non-singular terms on crack branching at low crack tip speeds. In this section, the considered methodology for the simultaneous detection of the crack path, the crack tip, the *SIF* and higher order terms from displacement fields is put forth. The extraction scheme in [Roux and Hild, 2006, Roux et al., 2009] is considered; it overcomes the inevitable sensitivity to noise found in previous methods; it can be indeed applied for extractions on curved cracks, and most prominently, is robust enough to be considered for analysing experimental displacement fields obtained via *DIC* on Ultra-High-Speed-High-Resolution images.

For a semi-infinite straight crack in a 2D elastic body subjected to a mechanical load, [Williams, 1957] proposes analytical solutions of symmetric (mode *I*) (Eq. D.1) and antisymmetric (mode *II*) (Eq. D.2) fracture modes. The elementary solutions are indexed by n , and i is the pure imaginary number $\sqrt{-1}$.

$$\Phi_I^n(r, \theta) = r^{n/2} \left(\kappa e^{in\theta/2} - \frac{n}{2} e^{i(4-n)\theta/2} + \left(\frac{n}{2} + (-1)^n \right) e^{-in\theta/2} \right) \quad (\text{D.1})$$

$$\Phi_{II}^n(r, \theta) = ir^{n/2} \left(\kappa e^{in\theta/2} + \frac{n}{2} e^{i(4-n)\theta/2} - \left(\frac{n}{2} - (-1)^n \right) e^{-in\theta/2} \right) \quad (\text{D.2})$$

The displacement field for a stationary crack around its tip can be written as:

$$u(r, \theta) = \sum_{k=I,II} \sum_{n=-\infty}^{\infty} a_k^n \bar{\Phi}_k^n(r, \theta) \quad (\text{D.3})$$

r and θ are the polar coordinates in the local frame of the crack tip (x'_1, x'_2) . κ is the Kolossov's constant. $\bar{\Phi}_k^n$ are the projection of Φ_k^n onto the (x_1, x_2) coordinate system, a_k^n represent different coefficients in the solution, i.e., for $n = 1$, a_I^1 relates to K_I , and a_{II}^1 relates to K_{II} . Following [Roux and Hild, 2006, Roux et al., 2009], the displacement fields $\underline{u}$ -whether experimentally or numerically obtained-, are projected onto what is known as a truncation of the Williams' series [Williams, 1957]. The solutions that are used for projecting the displacement fields and extracting the fracture parameters are truncated between $n = n_m = -3$ and $n = n_M = 7$ lowering the degrees of freedom of the inverse problem while maintaining a family of solutions that contains sufficient information about the crack features:

- $n = 0$, rigid body translation,
- $n = 1$, asymptotic terms (K_I, K_{II}) ,
- $n = 2$, T - stress and rigid body rotations,

In practice, especially in the experimental case, potential non-linear behaviour (plasticity, damage) close to the crack tip takes place. Since the methodology is based on an elastic description of the solid, only the mechanical behaviour outside a confined zone near the crack tip (Figure D.1) should thus be studied. This bridging of the far-field elastic loading to the local crack tip happens without any issues regarding probable non-linear behaviour near the crack tip.

D.2 SIF Extraction procedure

The extraction as proposed [Roux and Hild, 2006, Roux et al., 2009] proceeds as follows:

- (i) a crack path is proposed - in the numerical simulations the crack path is easily tracked thanks to the damage variable α . During actual experiments, crack path is obtained from images of the deformed sample transformed back to the Lagrangian configuration (see e.g. [Vinel et al., 2021]).
- (ii) the size of the pacman-shaped extraction domain is defined by a circular area of radius r_{ext} from which a small band of width r_{int} is removed around the crack tip (Figure D.1).
- (iii) the choice of the loading conditions (plane strain/plane stress) through κ is made. It's noted that κ can be added as a degree of freedom of the problem further validating the choice on the loading conditions.

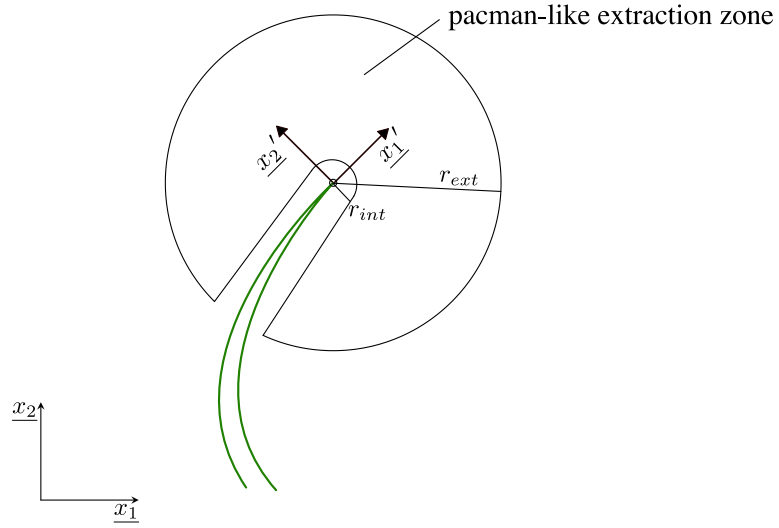


Figure D.1 – the pacman-shaped extraction domain

Throughout the extraction, the elastic crack tip position is updated using the first super-singular term $n = -1$, and the instantaneous *SIF* and *T-stress* are detected. The crack tip velocity v_c can be calculated consequently.

THEORETICAL ASPECT OF THE INERTIAL IMPACT TEST

This Appendix gives the reader more insights on the theoretical aspect of the global impact phenomena as the projectile hits the waveguide on which the specimen is mounted. Figure E.1 shows the interaction between the projectile, the waveguide and the sample, via a Lagrange representation of the impact, assuming that the projectile, waveguide and the specimen are made of the same material and that stress-waves travel at c_d inside each of them.

§ E.1. **Drawing the Lagrange representation of the impact:** a unidimensional wave propagation analysis in stepped rods is considered. The respective cross sections of the rods are modified to correspond to the cross-sections of the components of the ensemble. Initial velocity $V_{proj} = 30m/s$ condition is applied on the rod corresponding to the projectile, to mimic the experimental impact. FE analysis identifies the expected loading histories. Since the actual propagation is tridimensional, correction would be required on the Lagrange representation (Figure E.1) to accurately model the three-dimensional stress-wave propagation and interactions with the boundaries.

§ E.2. **Reading a Lagrange representation of wave interactions:** at fixed time, the horizontal line gives the state of the stress inside the system. The slopes of the showed lines actually represent the inverse of the speed of the stress wave, i.e., $1/c_w$ where c_w , $w \equiv d$ if longitudinal waves are considered and $w \equiv s$ if shear waves. It's noted that this representation also gives approximations on the loading/contact times.

Generally, several zones of interaction can be identified:

1. The projectile of length $80mm$ travels at $V_{proj} = 30m/s$. It hits an immobile waveguide at $t = t_1$ of same length on which a sample is mounted.
2. Directly after impact, two similar compression waves (dark blue) are generated in each element, and they propagate away from the impact surface. A clean impact is

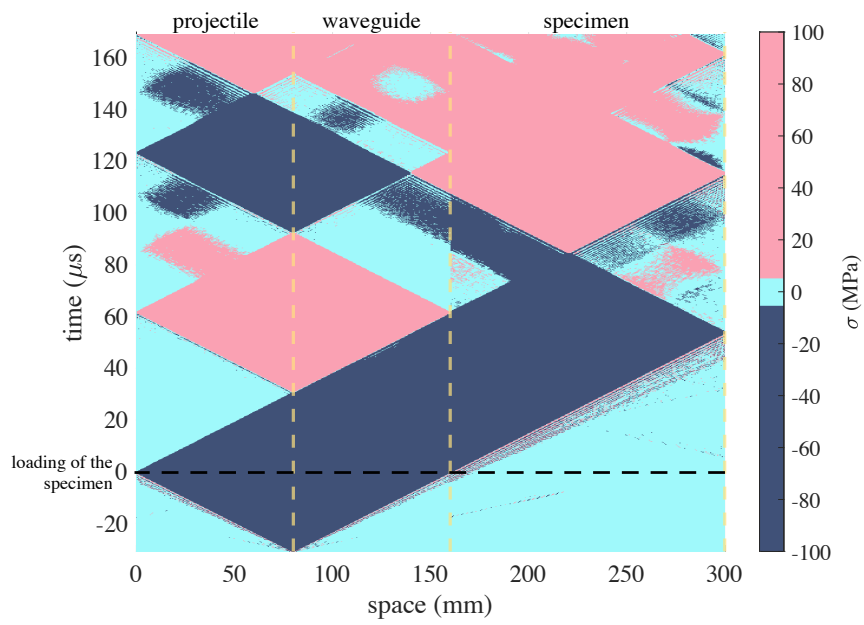


Figure E.1 – Lagrange representation of the inertial impact tests

assumed and the stress waves travel at c_d .

3. At $t=t_1 + 80mm/c_d$, the compressive stress waves in each rod reach the opposed surface. In the projectile, the boundary is free, and the compressive wave is reflected and returns inside the projectile as a tensile wave. The overlapping of the compressive and tensile waves gradually unloads the projectile (sky blue) until discharged. In the waveguide however, a part of the stress wave travels through the glue to the specimen and another part is reflected from the boundary as a tensile wave that partially unloads the waveguide for the previously mentioned reasons.
4. The specimen is now loaded in a compressive wave (dark blue colour).
5. At $t=t_1 + 2 \times 80mm/c_d$, the projectile is totally unloaded. The contact between the waveguide and the projectile is broken (bittersweet colour).
6. The compressive stress wave inside the specimen reaches the free boundary of the hole and is reflected back as a tensile wave that re-enters the compressed projectile. A range of mixed complex wave interactions happen afterwards.

Of course, the main interest is drawn to the last Point 6 corresponding to the stress-waves propagation inside the sample and their interaction with the geometry of the sample and the induced crack paths.

EXPERIMENTAL AND IMAGING SETUP OF THE INERTIAL IMPACT TEST

In this appendix, the experimental and imaging setup considered to capture the dynamic crack propagation, e.g., crack initiation, crack branching, stress-wave propagation, etc. are presented. Information already available in Chapter 5 are recalled.

F.1 Experimental setup and description of the test bench

The sample is laser-cut from a commercial PolyMethyl Methacrylate (PMMA) manufactured by Arkema. A synthetic speckle pattern is laser-engraved into the sample following [Vinel et al., 2021] (for the application of the *DIC* procedure).

The laser's beam diameter ($d_{laser} = 200\mu m$) is taken into account for the dimensioning. The pre-crack's width matches the beam's.

The projectile and the waveguide are machined from a polyoxymethylene (POM) cylinder of diameter $d_{proj} = d_{wg} = 40mm$; both are $80mm$ long. POM is used because it has similar material properties as PMMA

- The specimen is mounted to the waveguide ③ with the help of a machined wooden sleeve. It's then glued before removing the sleeve.
- The ensemble is systematically positioned on a PMMA support bed ④ at the end of the gun to secure the proper alignment with the projectile at the moment of impact (mounted on optical positioners ④).
- A projectile is fired by a gas gun ① to reach a velocity of V_{proj} just before the impact. The sudden expansion of the gas inside the barrels is what impels the projectile towards the waveguide.

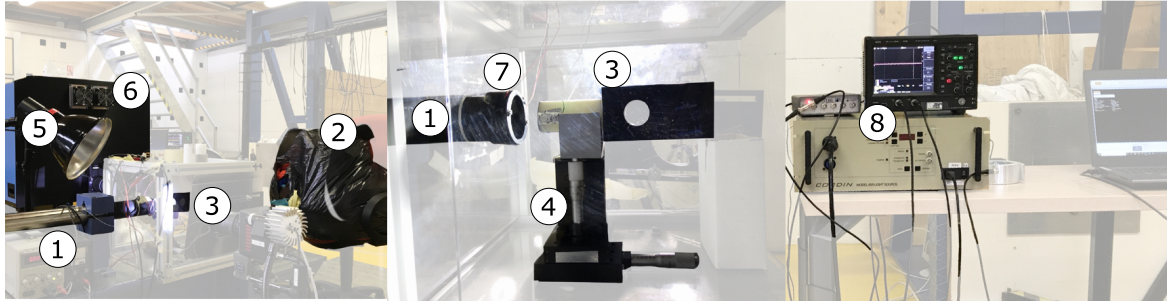


Figure 5.4 - Experimental set-up for the inertial impact tests

- The test is recorded with a Cordin Model 580 ⑥, *DIC* procedure is then applied (more in the next section)

A shock absorber ② is needed to neutralize the impact of the $0.12kg$ travelling at $\sim 30m/s$ from the gun end.

The purpose of using a waveguide instead of directly having the projectile impact the specimen is to ensure cleaner compressive waves at the boundary of the specimen, from one side, and holding the sample while keeping all other boundaries free.

A photo of the test bench can be found in Figure 5.4. One identifies:

1. The gas gun
2. The shock absorber
3. The specimen mounted on the waveguide
4. The PMMA support bed on the optical positioners
5. The flash lights
6. The UHS-HR camera: the Cordin Model 580
7. A light-gate: the SPX1189 series Honeywell infrared sensor
8. The delay generator (to synchronise the flashes)

To capture the extraordinary phenomena happening in vicinity of high velocity cracks, a highly resolved rotating mirror camera was used: the Cordin Model 580.

- The Cordin Model 580 ⑥ is set to capture a total of 78 images at $400k\ fps$ with a resolution of $3296 \times 2472px$.
- To provide enough lighting for the camera sensors, additional lighting is provided by two Pro-10 Profoto flashes ⑤ ($2 \times 2400J$ provided in $1000\mu s$).

At such $400k$ fps and $3296 \times 2472px$ resolution, the camera records the entire test ③: from the first compressive waves induced by the impact to the total failure of the specimen (about $200\mu s$, 78 frames). A schematic representation of the triggering of the camera and flashes (Figure 5.4) is plotted in Figure F.1.

- The flashes are triggered via an infrared light-gate system (SPX1189 series Honeywell) ⑦ mounted at the end of the gas gun ①. When obscured by the projectile ②, it sends a $5V$ TTL signal ① (rise time = $5\mu s$). The signal is then delayed by $200\mu s$ ② via a delay generator ③ before igniting the flashes ④. *The delay takes into account for the air-travel time of the projectile (from the outlet of the gas gun to the impact) + the time it takes the stress waves induced in the waveguide to reach the specimen - the warm-up time of the flashes* (Figure F.1).
- Two pieces of aluminium film are bonded onto the waveguide ③ and connected to a circuit (open) between a $5V$ generator and the camera trigger ⑥, so that when the projectile hits the waveguide, it contacts ④ both pieces of film closing thus the circuit and providing the triggering signal for the camera.
- The camera is then triggered with a delay of $40\mu s$, which corresponds to the time the stress waves (generated at the impact with the projectile) take to reach the boundary of the specimen through the waveguide.

F.2 On the mesh and DIC parameters

Since a crack is propagating in the sample during the test, the DIC requires meshing the samples in two steps, (see [Vinél et al., 2021] for more details). An unstructured mesh (of size $h = 2mm$) with twin nodes along crack paths is considered (from the final frame, in the un-deformed configuration). The mesh is refined in the zone near the crack path to $h_d = 1mm$. At $400k$ fps with a resolution of $3296 \times 2472px$, the finite element size is around $22px$ on average in the refined region, $44px$ elsewhere. (each pixel corresponds to $47\mu m$).

We also recall some remarks regarding the processing of DIC data:

Remark F.1. *Unlike in statics where standard cameras are used and where DIC yields accurate measurements, in dynamics, especially when recording with an UHS-HR rotating camera at $400kfps$, neat imaging cannot be achieved. Despite the application of the novel*

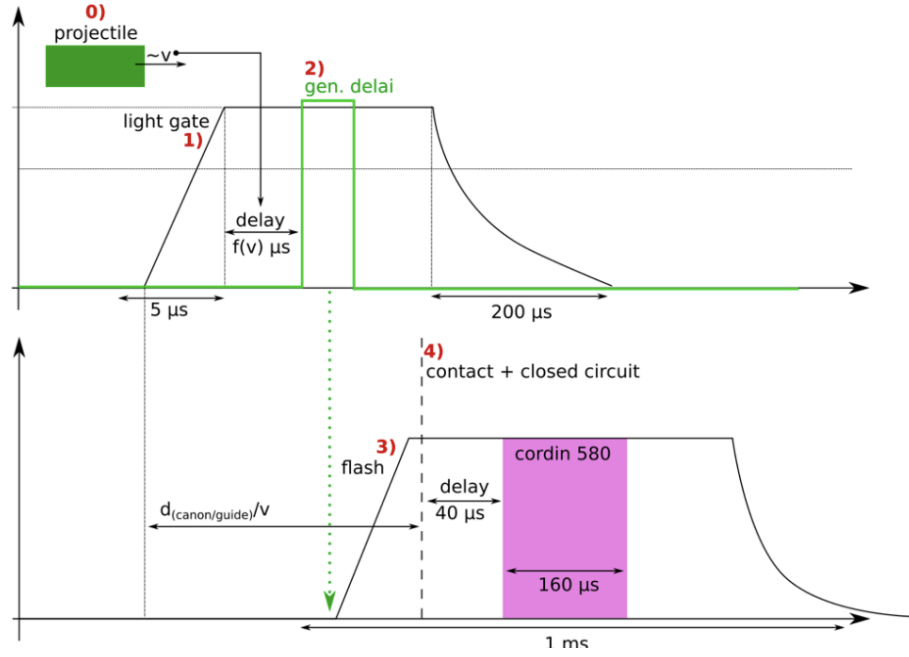


Figure F.1 – Imaging setup: automatic triggering of the camera and the flashes

calibration method from [Vinel et al., 2021] to suppress apparatus induced distortions, residual distortions may remain introducing a bias in the DIC measurements.

Remark F.2. The displacement fields are filtered in time with a Savitzky Golay (kernel size= 5 frames, order 2) filter to smoothen the first derivative (velocity fields); moreover, spatial noise is filtered-out via a Tikhonov regularisation of the DIC problem.

Remark F.3. The strain-rate fields are derived by spatial differentiation of the velocities; velocities are derived from temporal differentiation of the displacement fields.

Remark F.4. The time origin ($t = 0$) corresponds to the camera trigger.

Remark F.5. The initiation and the bifurcation frames are determined from the opening of the crack lips (twin nodes along the crack path) in the images from the UHS-HR camera.

Remark F.6. The opening of the crack lips along the crack path (twin nodes along the crack path) allows the computation of an apparent crack tip speed.

TAF2 SAMPLE: *DIC* FIELDS AND *SIF* RESULTS

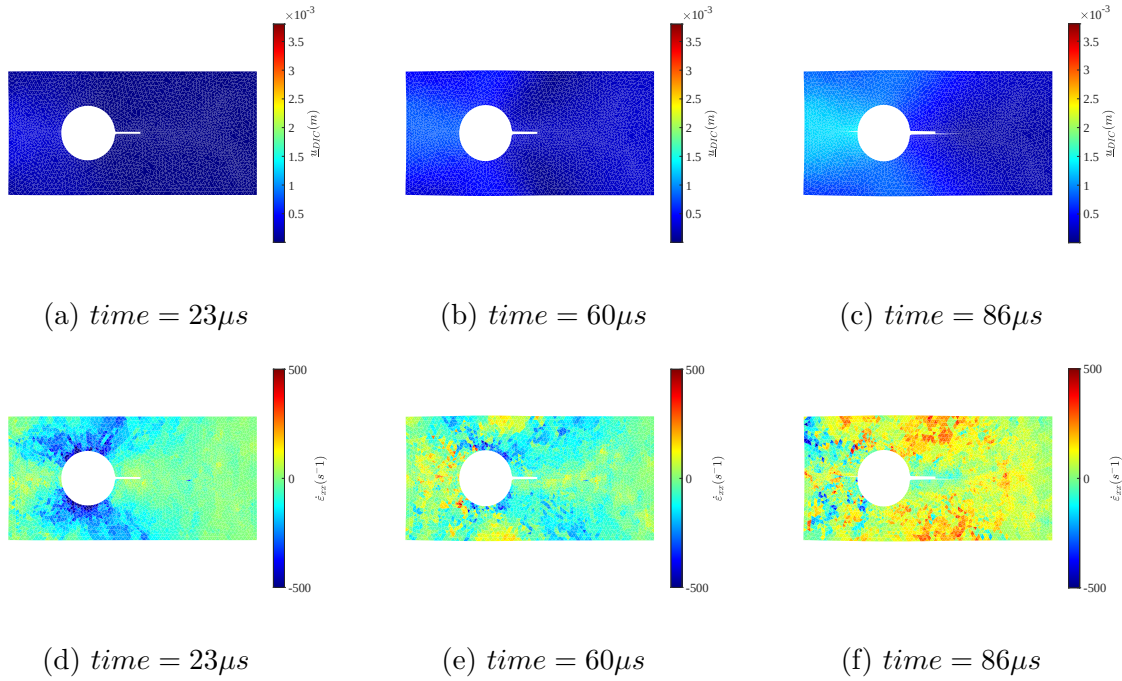


Figure G.1 – Sample TAF2 - *DIC* displacement fields (up) and longitudinal strain rates (down) at three time steps. A Savitzky Golay (kernel size= 5 frames, order 2) filter smoothens the displacements' first derivative (velocity fields). Spatial noise is filtered-out via a Tikhonov regularisation of the *DIC* problem

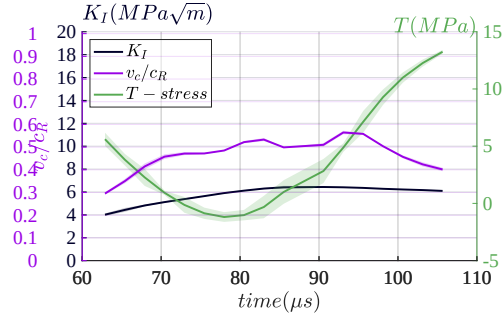


Figure G.2 – Sample TAF2 - *SIF*, the higher order term $T - stress$ and the crack tip speed. The error-bar corresponds to the sensibility to the extraction zone [Roux and Hild, 2006, Roux et al., 2009]

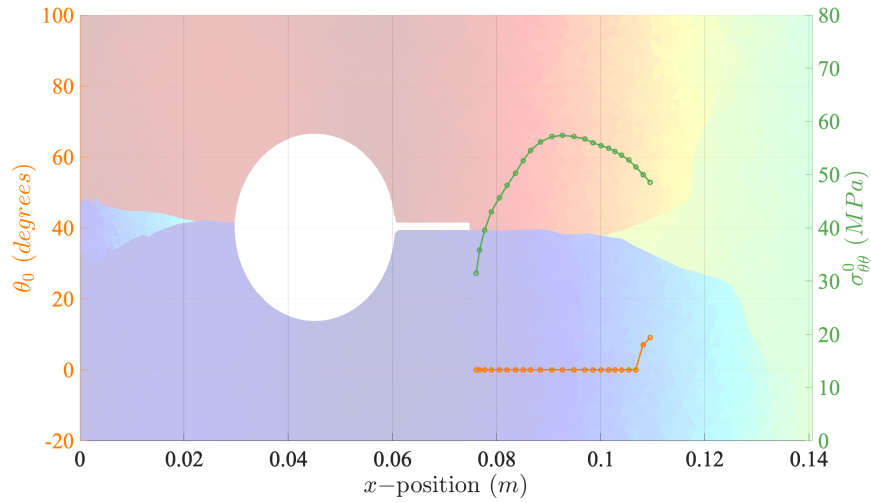


Figure G.3 – Sample TAF2 - Evolution of the predicted fracture direction θ_0 along with the maximum circumferential stress computed at $r_c = 2mm$. The modification of the fracture angle at the position of branching and the evolution of $\sigma_{\theta\theta}^0$ mirror the branching.

T3DE SAMPLE: *DIC* FIELDS AND *SIF* RESULTS

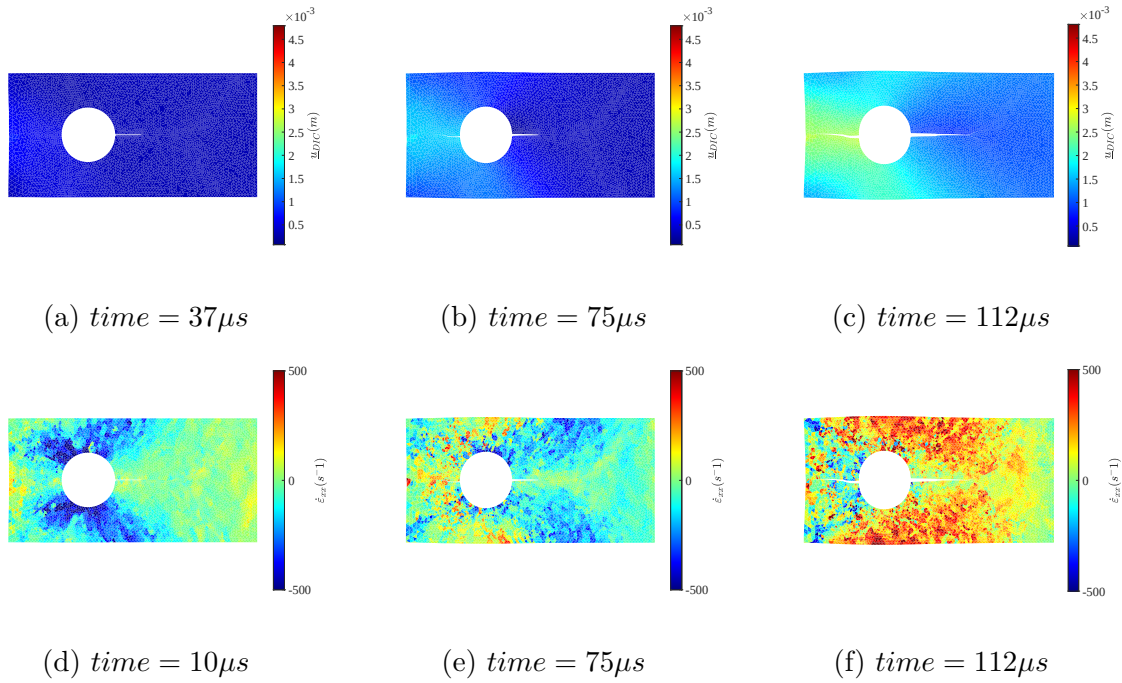


Figure H.1 – Sample T3DE - *DIC* displacement fields (up) and longitudinal strain rates (down) at three time steps. A Savitzky Golay (kernel size= 5 frames, order 2) filter smoothens the displacements' first derivative (velocity fields). Spatial noise is filtered-out via a Tikhonov regularisation of the *DIC* problem

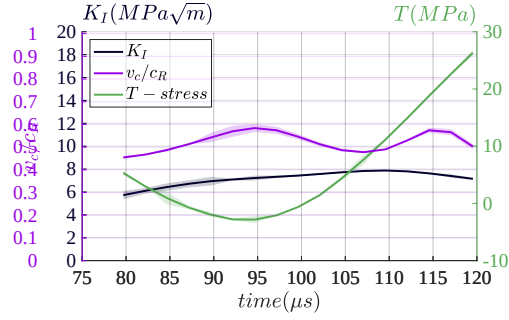


Figure H.2 – Sample T3DE - *SIF*, the higher order term $T - stress$ and the crack tip speed. The error-bar corresponds to the sensibility to the extraction zone [Roux and Hild, 2006, Roux et al., 2009]

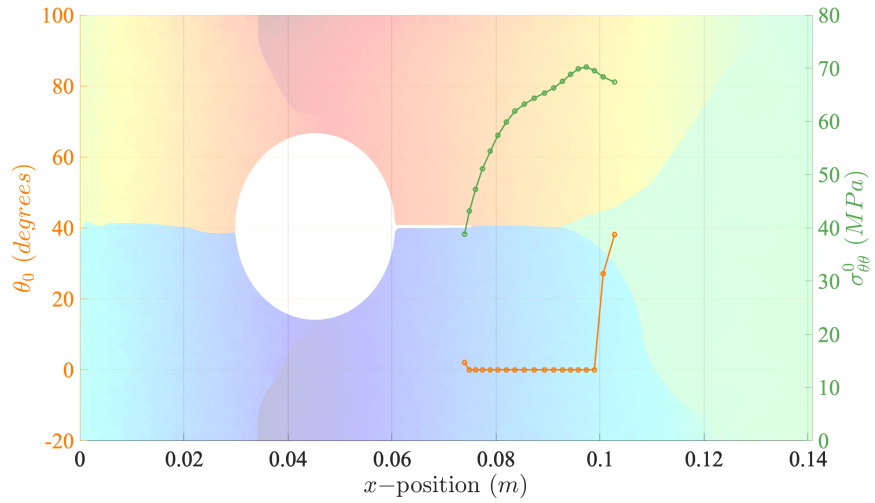


Figure H.3 – Sample T3DE - Evolution of the predicted fracture direction θ_0 along with the maximum circumferential stress computed at $r_c = 2mm$. The modification of the fracture angle at the position of branching and the evolution of $\sigma_{\theta\theta}^0$ mirror the branching.

THOM SAMPLE: *DIC* FIELDS AND *SIF* RESULTS

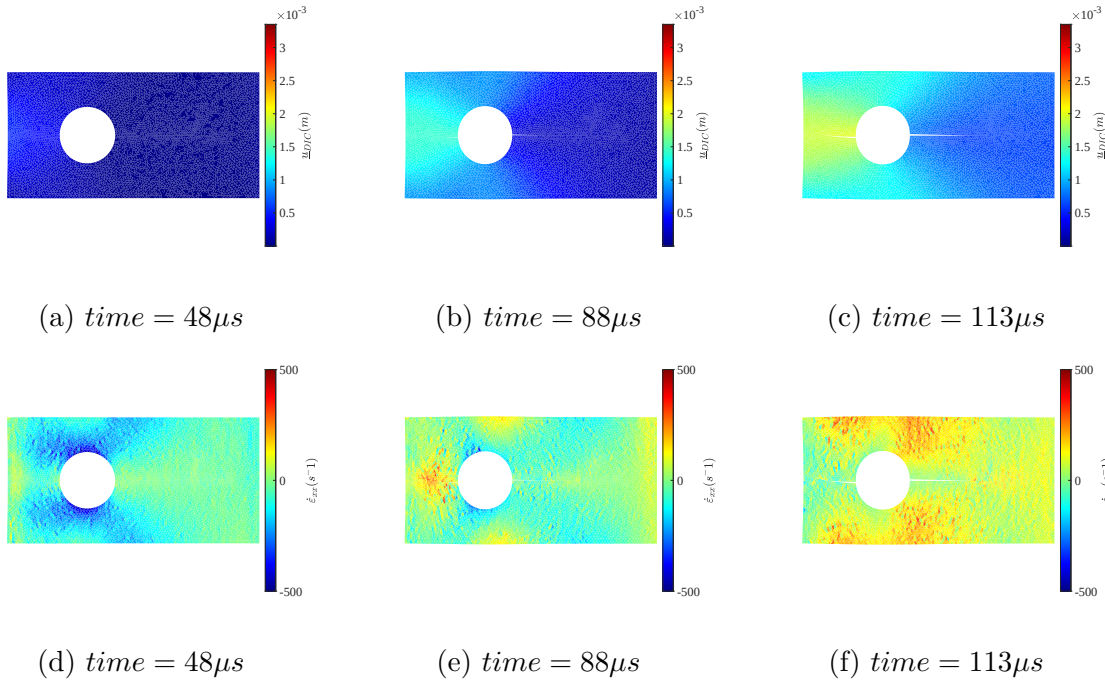


Figure I.1 – Sample THOM - *DIC* displacement fields (up) and longitudinal strain rates (down) at three time steps. A Savitzky Golay (kernel size= 5 frames, order 2) filter smoothens the displacements' first derivative (velocity fields). Spatial noise is filtered-out via a Tikhonov regularisation of the *DIC* problem

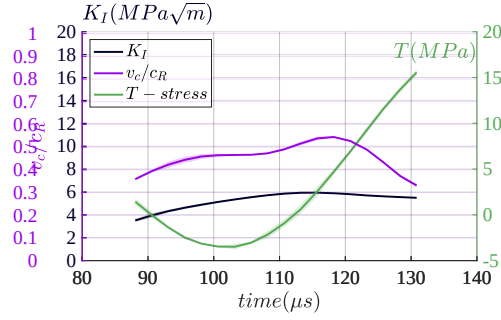


Figure I.2 – Sample THOM - SIF , the higher order term $T - stress$ and the crack tip speed. The error-bar corresponds to the sensibility to the extraction zone [Roux and Hild, 2006, Roux et al., 2009]

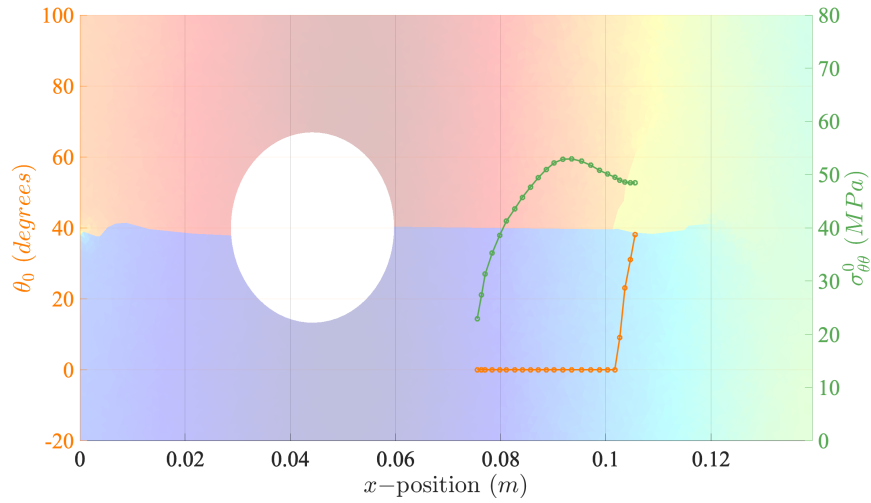


Figure I.3 – Sample THOM - Evolution of the predicted fracture direction θ_0 along with the maximum circumferential stress computed at $r_c = 2mm$. The modification of the fracture angle at the position of branching and the evolution of $\sigma_{\theta\theta}^0$ mirror the branching.

INFLUENCE OF r_c ON THE MATERIAL (IN)STABILITY MAP

This appendix covers the influence of the critical distance r_c on the (in)stability map of an arbitrary material: we recall that r_c is considered to be the distance at which crack growth occurs when incorporating higher order terms (e.g., $T - stress$).

Consider three arbitrary materials of mechanical properties equivalent to the ones in Table 5.1. Let $K_{IC} = 1.66 MPa\sqrt{m}$, and $m = 0.465$ the parameters representing the fracture behaviour following [Kanninen and Popelar, 1985]’s empiric law (5.7).

Assume the critical distance r_c for each material is different ($r_c = 2mm, 500\mu m, 8mm$), e.g., due to microstructural defects distribution. Figure J.1 shows the limiting boundary between a stable crack growth and an unstable one for each of the materials.

The boundary divides the $(v_c - T - stress)$ space into a zone where the direction of crack growth is along the extension of the crack ($\theta_0 = 0^\circ$), and a zone where $\theta_0 > 0$. This yields a well-defined curve separating stable and unstable crack growth.

The following observations can be drawn:

- At $T - stress = 0$, the classical solution [Yoffe, 1951, Freund and Hutchinson, 1992] is recovered independently of the distance r_c .
- For smaller r_c , the crack withstands larger $T - stress$ without branching.
- For larger r_c , the stability is improved at high crack tip speeds under larger negative $T - stress$.
- A negative $T - stress$ does not prohibit branching, even though it ensures more stability large crack tip speeds.

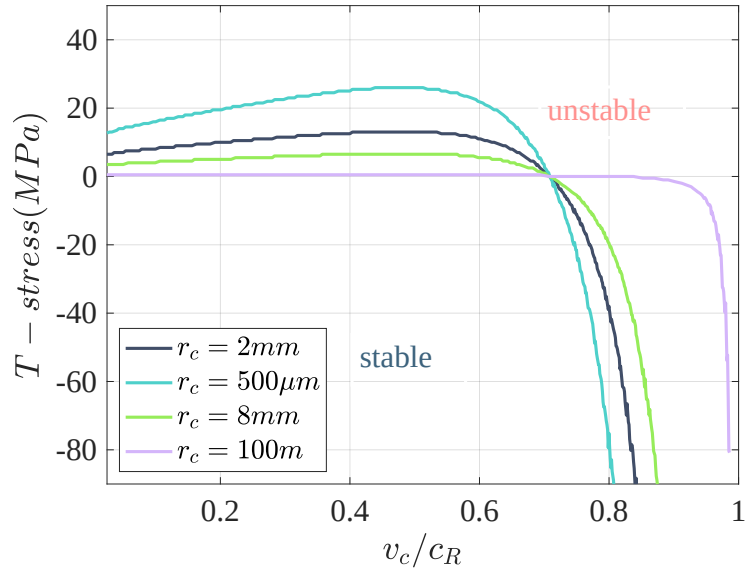


Figure J.1 – Influence of r_c on the material (in)stability map. A synthetic $r_c = 100\text{m}$ is added to validate the limiting velocity at $v_c = c_R$.

PHASE-FIELD SIMULATION OF THE INERTIAL IMPACT TEST: VALIDATION OF THE MODEL

K.1 Introduction

After successfully assessing the role played by $T - stress$ on crack (in)stabilities and crack branching on a novel experimental configuration, and after building the material (in)stability map that shows the loadings under which a crack growth can be stable or unstable, we check the ability of the phase-field model presented in Section 1.4 to replicate experimental crack propagation of the inertial impact test, in which, as we've seen, the stress waves play a crucial role in the crack path history.

We first recall the ingredients of the phase-field model used, then the material properties considered in the simulation.

It is assumed that the sample exhibits linear elastic behaviour. Details about the identification of the the elastic properties by taking the viscoelastic effects into account are given in Section 5.2.7.

The boundary condition (the impact) is then showcased, it's modelled thanks to the full-field measurements of *DIC*.

'*Post-mortem*' results of the phase-field simulations are presented, and the ability to accurately replicate the branching is noted. Although '*post-mortem*' comparison with the experiment shows accurate prediction of the crack patterns and branching angles, we'll see (on the (in)stability map) (Figure 5.15) how the phenomenon leading the fracture is not the same as in the experiment (in the experiment it's mainly a running crack under positive $T - stress \simeq 10MPa$).

We show how phase-field modelling, although pretty accurate in predicting crack patterns, are haphazard in terms of replicating crack history and tip speeds. From the

analysis of the fracture angle, we see how the instability is initiated at early stages in the propagation where the crack is at relatively high crack tip speeds typically as the damage band in phase-field starts broadening.

K.2 The phase-field parameters

Table 5.2 resumes the overall model and material parameters considered in this simulation of the inertial impact test.

Time stepping	Explicit ([Li et al., 2016b])
Crack density function	Quadratic, Equation 1.3 ([Miehe et al., 2010a])
Strain split	Orthogonal ([Nguyen et al., 2020b])
Plane strain assumption	
Boundary condition	Experimental $\underline{u}$ [Vinel et al., 2021]
E (Young's Modulus)	6GPa Section 5.2.7
ν	0.3
g_c	1100J/m ²
l_c	2 $\times$ mesh size = 2 $\times$ h = 1mm ([Nguyen et al., 2016])
c (threshold)	1

Table K.1 – Table 5.2 - Overall phase-field model and material parameters considered in this simulation of the inertial impact test.

K.3 The boundary condition

Accurate determination of the boundary condition is crucial for the phase-field simulation to accurately replicate crack patterns.

From the *DIC*, the full-field kinematics allow the capture of the experimental displacement fields around the boundary. This boundary displacement condition is then prescribed to the loaded boundary phase-field simulation.

Figure K.1(a) shows the impacted boundary, i.e., the surface on the left-hand side of the specimen, on which the waveguide is glued to the specimen. The other boundaries are free [Pierron et al., 2014]. From *DIC*, the evolution of the average u_1 displacement of the boundary and its velocity (average at each time step along the nodes of the boundary) in time are shown in Figure K.1(b) (for visualisation purposes).

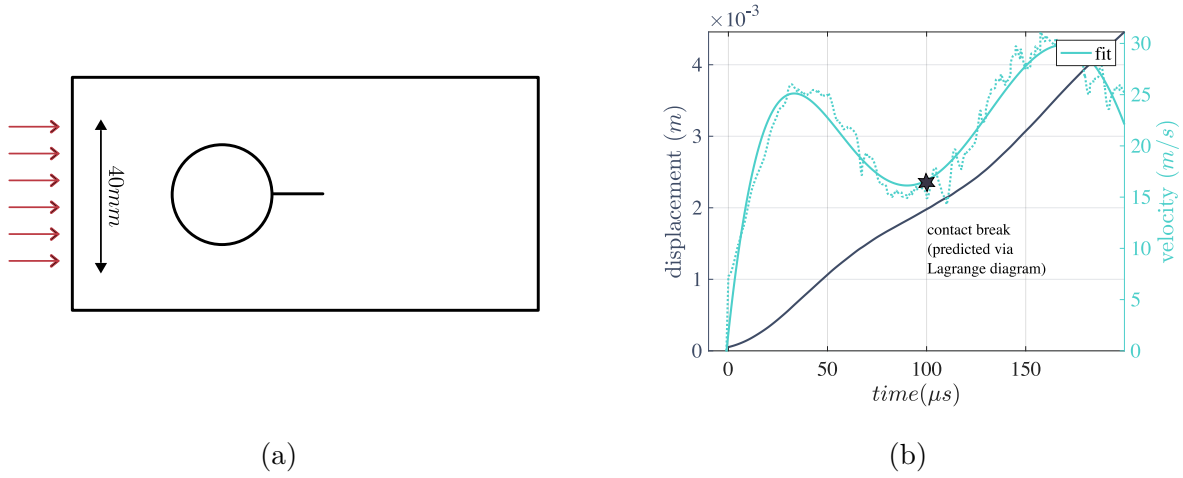


Figure K.1 – Boundary condition for the inertial impact test. The displacement and velocity of the experimental boundaries are obtained from *DIC* and imposed on the simulation. The time from which the contact between the waveguide and the specimen is broken is predicted from Appendix E and noted on the plot

Remark K.1. Attention is drawn to imposing both displacement components u_1 and u_2 of the *DIC* in the simulation, to accurately assess the slight dissymmetry in the experimental crack pattern (Figure 5.5).

Since the simulation's Finite Element Mesh is much finer, interpolation of the nodal displacement was required.

Remark K.2. In the inertial impact test, as contact is established between the projectile and the waveguide, compressive stress-waves are generated in each element, and they propagate away from the impact surface. The compressive stress waves reach the specimen, the boundary is now loaded. The return travel of the stress-waves (tensile, reflected from the free boundaries) along the waveguide and specimen breaks contact (Appendix E). This contact breaking should be taken into account in the boundary condition, i.e., the displacement boundary condition from *DIC* should be removed at the time of contact loss. However, the finely synced material properties and stress-wave propagation removes the need for freeing the boundary of impact when the contact is lost, as the simulation perfectly reproduces the big lines in the stress-wave propagation.

K.4 Simulation results

K.4.1 On the crack patterns

Figure 5.17 shows both experimental (*DIC* measurements) and simulation results (phase-field simulations) of the inertia impact test TAF1. The crack patterns are clearly reproduced by the phase-field simulation: the branching position and the branch turning are accurately predicted.

We note the widening of the damage band in the simulation before the moment of branching, similarly to other phase-field simulations reported in [Borden et al., 2012], [Schlüter et al., 2014], and to non-local integral damage model [Pereira et al., 2017]¹. To further investigate the branching and damage band widening, the (in)stability criterion is applied. Beforehand, let us briefly describe the crack path history and crack tip speeds from the simulation and compare them with the experimental results from *DIC*.

K.4.2 On the crack tip speeds

In Figure 5.18, we superpose the crack tip velocities from the simulation and the crack tip velocities obtained experimentally. Even though the crack patterns are accurately reproduced, the crack path history and crack tip speeds are not.

This can be caused by various reasons, possibly and not exclusively;

- Viscous effects: even though PMMA is THE model material for in-lab studying the brittle elastic failure, its viscous behaviour has already been documented and quantified, e.g., in [Seghir and Pierron, 2018].
- Wrong phase-field parameters: as seen in Chapter 1 and Appendix A, comparable crack paths can be obtained for different combinations of parameters l_c , g_c and c , however, discrepancy in the crack tip speeds are often present. With the contribution to the phase-field modelling in Chapter 1, the parametrisation of the threshold (Chapter 1) allows for a triplet of parameters to be optimised for accurately reproducing experimental scenarios by elegantly balancing the energy dissipation, energy release-rate and fracture strength. This yields more freedom in the choice. Even

1. From a more physical point of view, damage widening could be the signature of roughening of the crack surface experimentally observed to occur prior to branching [Ramulu and Kobayashi, 1985]. [Bleyer and Molinari, 2017] showed that the micro-branching process is indeed a three-dimensional instability and is directly linked to surface patterns observed prior to macro-branching in PMMA [Sharon and Fineberg, 1996].

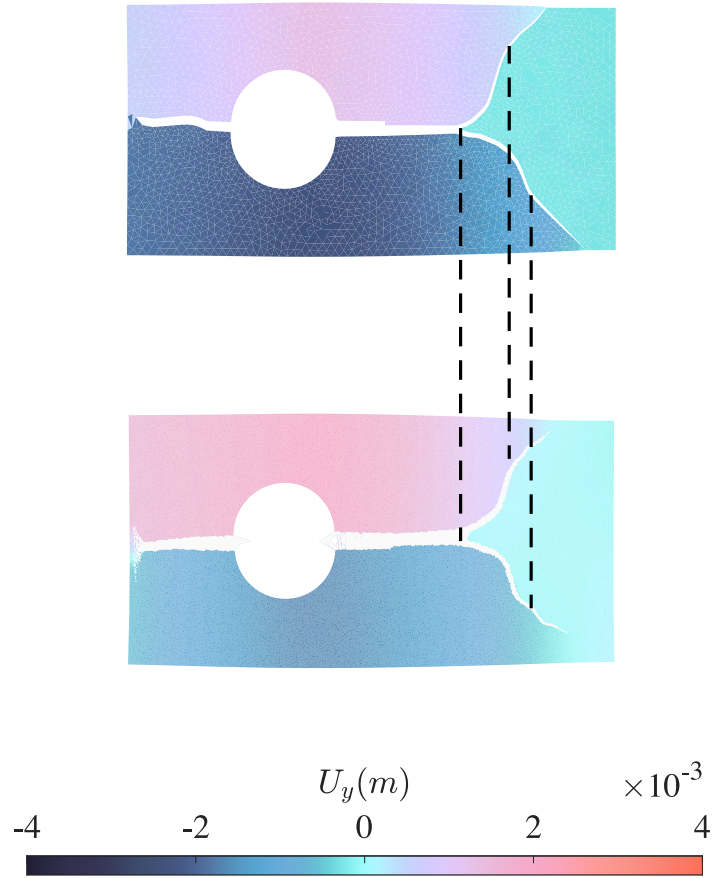


Figure K.2 – Figure 5.17 - *DIC* displacement field (up) and phase-field simulation results (down) showing accurate prediction validating the dynamic phase-field model and accurately reproducing the crack patterns. The points where the phase-field damage $\alpha \geq 0.99$ are removed to mimic crack opening.

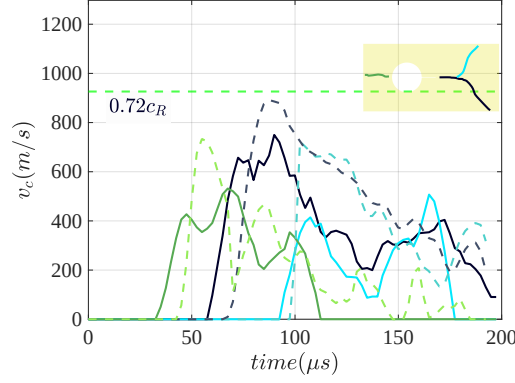


Figure K.3 – Figure 5.18 - Comparison of the experimental and numerical (phase-field simulation) crack tip speeds. Dashed lines correspond to the crack-tip speeds estimated from the phase-field simulation (Appendix B), full lines correspond to the apparent experimental crack tip-speeds previously reported in Figure 5.7

though this parametrisation offers a wider range of material behaviour, it is crucial to span the triplets in the search for the optimum phase space.

Remark K.3. *Without the UHS-HR imaging and the cutting edge DIC algorithms, the obtained simulation results would be satisfactory. However, these technological advancements offer sound ground for a more rigorous estimation of the phase-field parameters that should yield a more precise reproduction not only of the patterns, but also crack tip speeds and crack history.*

Next, we advocate instabilities on the phase-field simulation results based on the proposed method.

K.4.3 Crack branching analysis

Indeed, since only displacement fields are required for the analysis, the proposed scheme is readily applicable on displacement fields coming from numerical simulations.

$$\underline{u}_{SIMU} \rightarrow SIF, T - stress, \text{ crack tip position, and } v_c \rightarrow \underline{\sigma} \rightarrow \sigma_{\theta\theta} \rightarrow \sigma_{\theta\theta}^0 \ \& \ \theta_0$$

Figure 5.19 shows the estimations of the crack-tip speed, SIF and $T - stress$; the following observations can be drawn:

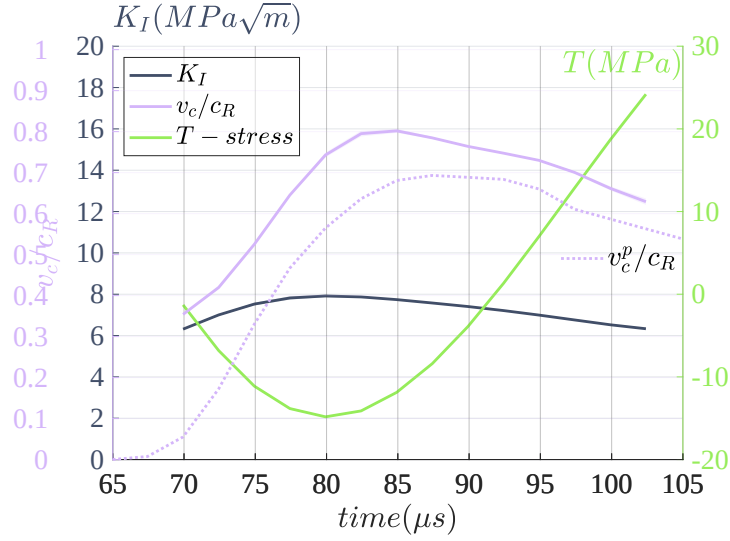


Figure K.4 – Figure - 5.19 *SIF*, the higher order term $T - stress$ and the crack tip speed in the simulation of the TAF1 sample test. The error-bar corresponds to the sensibility to the extraction zone [Roux and Hild, 2006, Roux et al., 2009]. The crack tip speed v_c^p corresponds to the one reported in Figure 5.18 computed from the phase-field, via Appendix B

- The estimations show similar trends to the experimental estimations.
- From $t = 70\mu s$ (crack initiation from the notch) to $t = 80\mu s$, K_{ID} increases from $K_{ID} = 6.28MPa\sqrt{m}$ to $K_{ID} = 7.91MPa\sqrt{m}$.
- The velocity of the elastic crack tip on the other hand reaches a maximum $v_c = 0.8c_R$ at $t = 85\mu s$. Afterwards, the crack tip starts decelerating until it reaches $v_c \simeq 0.72c_R$ at the moment of branching (branching detected from Figure 5.18), around $t = 95\mu s$.

Remark K.4. *On the difference between the computed crack tip speeds: the phase-field model introduces a damaged zone in which the dissipative processes are diffused to regularise a sharp crack (via the length-scale l_c). The methodology proposed in Appendix D is founded on LEFM that suggests that all non-linear and dissipative processes are well confined to the near-tip vicinity. The equivalent elastic crack tip (extracted from Appendix D) would eventually not coincide with a phenomenologically captured crack tip (e.g., iso-curves of the phase-field), the equivalent elastic crack tip is expected to accelerate as the damage band widens/lengthens and dissipates energy. A delay/deviation between those two computed speeds is natural and as it comes from their inherent differences.*

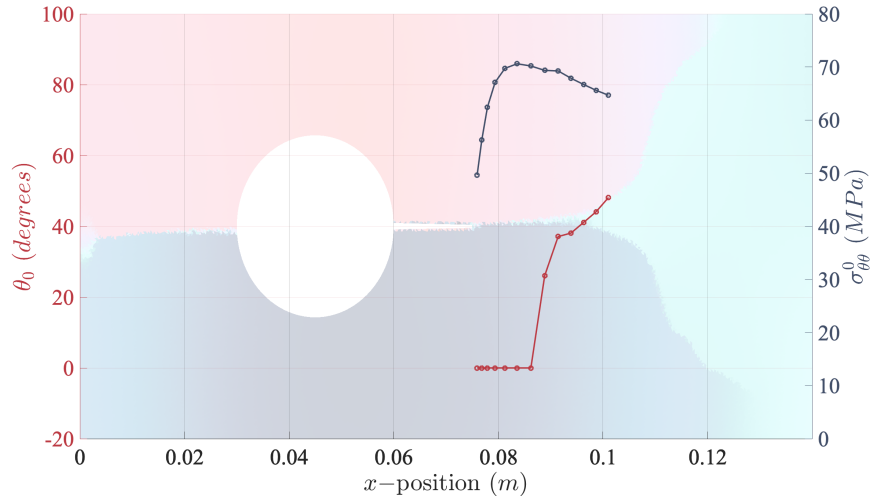


Figure K.5 – Figure 5.20 - Evolution of the predicted fracture direction θ_0 and the maximum circumferential stress $\sigma_{\theta\theta}^0$ computed at $r_c = 2mm$ in the phase-field simulation of the TAF1 sample (SIF , $T-stress$ and v_c from the numerical fields). The modification of the fracture angle θ_0 at the position of branching and the evolution of $\sigma_{\theta\theta}^0$ mirror the branching phenomenon

- Regarding the first higher order term, knowingly the $T-stress$, an initial decrease is observed to a negative $T-stress = -15MPa$ at $t = 80\mu s$. Afterwards, $T-stress$ rockets.
- As mentioned in Remark 5.2, neat imaging could not be achieved. Despite the application of the novel calibration method from [Vinel et al., 2021], residual distortions may remain introducing a bias in the DIC measurements. An estimation of potential biases hiding within the SIF , v_c and $T-stress$ identification showed discrepancies of $1MPa\sqrt{m}$, $0.1c_R$ and $3MPa$ respectively.

Remark K.5. From the experimental extraction on TAF1, the $T-stress$ remains positive, however a negative $T-stress$ is obtained in the simulation, the difference might find its roots in the difference of the crack tip speeds which makes the crack tip 'see' different loading/unloading histories. It's mentioned that in the other samples (Appendices G, H and I) a negative $T-stress$ is estimated after the initiation.

From here, we report the evolution of the direction of $\pm\theta_0$ at different positions of the crack tip inside the simulation in Figure 5.20. $r_c = 2mm$ is also considered consistently with the previous experimental findings.

Observing the obtained trend of θ_0 , we see the following:

-
- the fracture direction is first along the crack growth;
 - instabilities are predicted to occur earlier than in the experiment (a question arises: can these instabilities relate to damage band widening before branching?)
 - $\sigma_{\theta\theta}$ increases to around $70MPa$ and drops as the direction of propagation θ_0 becomes different than zero.

Simulation results on the (in)stability map

By superposing the crack propagation history $(v_c, T - stress)$ on the experimentally-built material instability map from Figure 5.15, we obtain the patterns in Figure 5.21.

Evidently, the history of crack propagation is much different than that in the experiments, even though it was accurately able to reproduce the crack patterns. The instability map shows the initiation of the propagation from the notch (circle marker) through the square marker corresponding to the damage band widening, until the moment of detection of branching (arrowhead). The map accurately shows a transition between the stable and unstable zones at the widening of the phase-field damage band: at negative $T - stress$ but at a high tip speeds. Afterwards, as the damage continues its straight propagation and reaches the branching position, $T - stress$ is closer to the experimental $T - stress$, but the crack tip speed is always larger. The predicted stress (Figure 5.21) is larger in the phase-field simulation. We believe that a more robust identification of the phase-field parameters is required to enable a better reproduction of the experimental crack patterns, crack tip speeds and eventually crack growth in the $(v_c, T - stress)$ space.

Remark K.6. *We're not sure how/if phase-field's length scale l_c is linked to this r_c , more investigations should be lead to further elaborate on this point.*

We summarise this application on the phase-field simulation by drawing the following points regarding:

- The phase-field model is able to accurately reproduce the crack patterns even in cases where the stress-waves play a major role on the crack propagation. However,
- UHS-HR imaging couples with the cutting-edge *DIC* algorithms allow a meticulous comparison of the crack propagation histories, and
- Unfortunately, the parameters herein used might not be the most accurate, as they are obtained by trial and error on the simulations to fit the pattern, the crack-tip speeds couldn't be recovered.

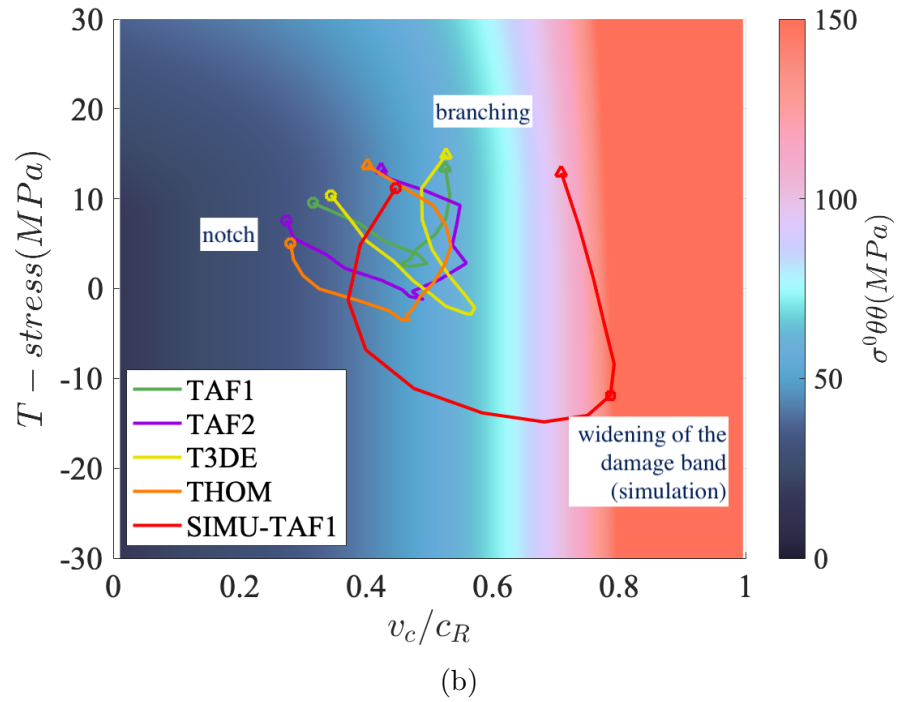
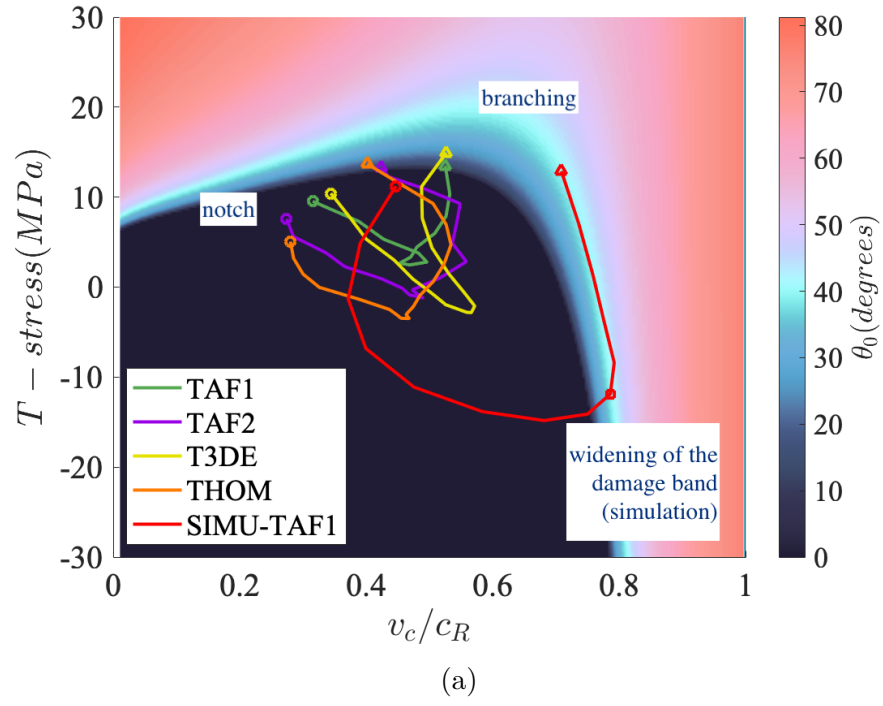


Figure K.6 – Figure 5.21 - (In)stability and maximum circumferential stress map of PMMA, constructed from experimental measurements and fitted to [Kanninen and Popelar, 1985]’s empiric law. The history of the crack propagation in each sample and in the phase-field simulation of TAF1 is shown

-
- The proposed methodology to assess the (in)stabilities shows how the history of the crack growth, despite the accurate replication of the crack patterns, is not reproduced.
 - Most prominently, the (in)stability map accurately predicts the crack branching and damage band thickening in the phase-field model as an interplay between the crack-tip speed and $T - stress$

Titre : Vers une analyse multi-échelle de la fissuration dynamique des matériaux architecturés

Mots-clés : Matériaux architecturés, coarse-graining, rupture fragile, rupture dynamique, branchement

Résumé : Durant ces dernières années, on a vu un intérêt de plus en plus marqué pour de nouveaux matériaux avancés appelés matériaux architecturés. On s'intéresse à la fissuration de matériaux architecturés dans lesquels la séparation d'échelle n'est pas toujours bien établie. Ceci se traduit par de fortes interactions entre le front de la fissure et l'architecture du matériau indépendamment de l'échelle considérée. De plus, sous chargements dynamiques, des ondes élastiques entrent en jeu et les interactions entre le front de la fissure, les ondes élastiques et la microstructure pilotent ensemble le comportement global de la structure. Dans cette thèse, trois types de matériaux architecturés (microstructures) sont considérés : un réseau de trous périodique et deux réseaux quasi-périodiques type Penrose. L'analyse est divisée en trois parties. Celle-ci permet donc une évaluation multi-échelle cohérente des propriétés effectives à la rupture des microstructures périodiques et quasi-périodiques. On montre ainsi l'inévitabilité de la prise en compte d'un milieu effectif non-homogène pour modéliser avec précision la réponse globale d'un matériau en tenant compte de sa sous-structure. En dynamique, une analyse de l'influence de l'architecture sur l'atténuation des ondes élastiques montre une meilleure performance des réseaux quasi-périodiques. De plus, pour comprendre le ou les mécanismes régissant le phénomène de branchement dynamique dans un milieu homogène, un critère basé sur la mécanique de la rupture dynamique est développé et validé sur une nouvelle configuration expérimentale où l'imagerie à haute vitesse et haute résolution est combinée à la corrélation d'images numériques pour capturer les phénomènes marquants. Le rôle incontestable que joue la contrainte T dans le branchement dynamique est mis en avant. Cette thèse fournit ainsi les outils nécessaires à une analyse multi-échelle de la rupture dynamique des matériaux architecturés. Pour étudier l'influence de la microstructure sur la propagation des fissures à différentes échelles, des simulations numériques de rupture sont analysées ; ces simulations montrent une meilleure résistance des matériaux quasi-périodiques à la propagation des fissures. De plus, on développe une approche de changement d'échelle "bottom-up" qui n'a pas recours à la notion de volume élémentaire représentatif.

Title: Towards a multi-scale analysis of dynamic failure in architected materials

Keywords: Architected materials, coarse-graining, brittle fracture, dynamic fracture, crack branching

Abstract: Architected materials are a rising class of materials that provide tremendous possibilities in terms of functional properties. Interest is drawn on the failure of architected materials in which scale separation ceases to exist. This directly translates to strong interactions between a crack tip and the architecture independently of the considered scale. Moreover, under dynamic loadings, stress-waves come into play and interactions between the crack-tip, the microstructure (architecture) and the stress-waves eventually pilot together the structural behaviour. In this thesis, three types of architected materials are considered: one periodic and two Penrose-type quasi-periodic lattices of holes. The analysis is broken into three parts. To study the influence of the microstructure on crack-propagation at different scales, numerical simulations of failure are analysed; they show improved resistance to crack propagation in the quasi-periodic materials. At the core of the work is also the development of a coarse-graining technique that requires no representative volume element. This technique allows for a physically consistent multi-scale evaluation of the effective failure properties of the architectures. The inevitability of the consideration of a non-homogeneous effective medium to accurately model microstructural effects at larger scales is highlighted. In dynamics, the influence of the architectures on the stress-wave attenuation shows improved attenuation properties of the quasi-periodic lattices. Moreover, to understand the mechanism(s) governing the dynamic branching phenomenon in a homogeneous material, a criterion based on dynamic fracture mechanics is developed and validated on a novel experimental setup where Ultra-High-Speed-High-Resolution imaging is combined with Digital Image Correlation to capture extraordinary phenomena. The unquestionable role of T-stress in dynamic branching is put forth. This thesis brings forth the necessary tools towards a multi-scale analysis of dynamic failure of architected materials.
