

# Development of materials criticality profiling methodology at product level

Yanya Jin

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Thèse de doctorat de l'UTT

# Yanya JIN

# Development of Materials Criticality Profiling Methodology at Product Level

Spécialité : Ingénierie Sociotechnique des Connaissances, des Réseaux et du Développement Durable

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pour l'obtention du grade de

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présentée et soutenue par

Yanya JIN

le 31 janvier 2017

Development of Materials Criticality Profiling Methodology at Product Level

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# ABSTRACT

Title: Development of Materials Criticality Profiling Methodology at Product Level

Jan. 2017

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#### M.A., UNIVERSITY OF TECHNOLOGY OF TROYES

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[Recently, several institutions have designated rare earths as critical resources after their supply disruption in 2010 which showed the importance of some materials to industries and governments. This fact also whipped up interest in the research on material criticality. Similar crises or issues can be found in the history although the concept of criticality was not the same as it is today. Situations like these will continue to happen in the future, even more due to the development of technology and society and the ever-increasing or new needs in raw materials. A better understanding of the mechanism of criticality will help us mitigate and prepare for such eventualities. A review work was first conducted in order to get a better understanding of the existing work in this research area and to see where more work is needed. Based on this review, three research gaps were identified. Firstly, most of the existing work uses pre-established critical materials or developed directly the evaluation methodology without providing at first a comprehensive analysis of what elements make materials critical and how (a diagnosis of criticality). Secondly, current work lacks evaluation methodology at product level (available to the public) whose results are more directly useful to corresponding companies. Those with scope of administrative area, a specific group of materials or technologies have already been worked on. Finally, the relation between the mechanism of criticality, the evaluation methodology and the solutions offered has not been established. Based on previous work, this thesis focuses on the two first research gaps and offers several ideas for the last one. Regarding diagnosis of criticality, the mechanism is illustrated under four dimensions: imbalance between supply and demand, importance of the material to product, supply accessibility and dynamic factors. A definition of criticality is also put forward. Considering the established mechanism as research core, a methodology to evaluate the criticality of materials at product level has been developed and is completed with a concrete and quantitative model. The methodology offers guidance on how to assess criticality and sets a framework for evaluation. The model illustrates a way to use this methodology through a tool that assigns a 'criticality score' to materials and shows how the score is contributed. The calculations were automated in Excel. Two applications, one for permanent magnet and the other for light emitting diode, were conducted to demonstrate and improve the methodology and the model. The thesis discussed limitations, observations and derived research work for future and concluded with indicating contributions.]

# **ABSTRACT (VERSION FRANÇAISE)**

# Titre: Développement d'une Méthodologie d'Évaluation de la Criticité des Matériaux au Niveau du Produit

#### Jan. 2017

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De nombreuses organisations ont récemment désigné les terres rares comme « ressources critiques ». Les impacts causés par la crise de ce groupe de métaux en 2010 ainsi que la plainte associée devant l'Organisation Mondiale du Commerce mettent en évidence l'importance des matériaux pour certaines entreprises ou certains pays, et ont conduit en un intérêt accru dans la recherche sur leur criticité. Des cas similaires peuvent être observés à travers l'histoire des civilisations même si la notion de criticité n'était bien sûr pas perçue de la même façon qu'aujourd'hui. Il est d'ailleurs possible d'anticiper que des crises liées à la criticité continueront à survenir dans le futur, peut-être même plus souvent, étant donné l'augmentation ou l'émergence des besoins en matières premières engendrée par les développements technologiques et sociaux. Une meilleure compréhension du mécanisme de la criticité nous aiderait à mieux nous y préparer. Cette thèse entend contribuer à cet objectif général. Elle s'ouvre par un état de l'art qui présente et évalue les travaux existants dans ce domaine. L'état de l'art met en évidence trois lacunes de la recherche sur la criticité des matériaux (une désignation de la criticité discrétionnaire ou une détermination de la criticité peu fondée sur un véritable diagnostic de criticité avant l'évaluation ; l'absence d'une méthodologie d'évaluation de la criticité au niveau produit en complément d'analyses régionales, sectorielles ou d'un groupe spécifique du métal ; le défaut de lien bien établi entre mécanisme de criticité, méthode d'évaluation et solutions proposées). En conséquence, et à partir du corpus de résultats existants, la thèse comble les deux premières lacunes et offre plusieurs pistes à l'égard de la troisième. Concernant le diagnostic de la criticité d'un matériau, la thèse propose de déterminer le mécanisme de criticité par quatre dimensions : le déséquilibre entre offre et demande ; l'importance du matériau pour le produit ; l'accessibilité de l'approvisionnement ; et les facteurs dynamiques. Une définition de la criticité est proposée. Le mécanisme de criticité étant au centre de la recherche, une méthodologie permettant de déterminer la criticité matérielle à l'échelle « produit » est développée et complétée par un modèle applicatif quantitatif. La méthodologie offre un raisonnement général pour conduire une étude de la criticité ; le modèle illustre une de ses possibilités d'être appliqué à des cas réels pour déterminer quantitativement la criticité (par un système de scores, dont les calculs sont automatisés sous tableur informatique). L'application du modèle à deux produits (l'aimant permanent et la diode électroluminescente) est présentée, qui permet d'éprouver et d'améliorer la méthodologie, ainsi que le modèle. Une discussion finale souligne certaines limites des travaux, des observations personnelles et quelques perspectives pour de futurs développements pendant qu'une conclusion résume les réponses aux questions de recherche et les contributions de la thèse.]

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# **ABBREVIATIONS**

# Abbreviations of organizations or general use

- A.D.: Anno Domini
- APS : American Physical Society
- MRS : Material Research Society
- **CF** : Companion metal Fraction
- CIS : Commonwealth of Independent States
- CMI : Critical Material Institute
- CN: China
- DOE : Department of Energy
- DTPA : Diethylenetriaminepentaacetic acid
- EC : European Commission
- EU : European Union
- GDP : Gross Domestic Product
- GII : Global Innovation Index
- GM: Germany
- GSC : Global Supply Concentration
- HDI : Human Development Index
- HHI : Hirfindahl-hirshmann Index
- IEA : International Energy Agency
- IMF : International Monetary Fund
- INSEE : Institut National de la Statistique et des Etudes Economiques
- IP : Impact Parameter
- ITA : International Trade Commission
- ITC : International Trade Commission
- JP: Japan
- KR: Korea
- LCI : Life Cycle Inventory
- LCIA : Life Cycle Impact Assessment
- LED : Light Emitting Diode
- MCPM : Materials Criticality Profiling Methodology
- MFA : Material Flow Analysis

NEDO : National Economic Development Office

NL: Netherland

NRC : Nation Research Council

PPI : Policy Potential Index

QWS : Quantum Wells

RE : Rare Earth

REE : Rare Earth Element

REO : Rare Earth Oxide

SCF : Société Chimique de France

UK : United Kingdom

U.S.: United States

USGS : United States Geological Survey

WGI-PV : Worldwide Governance Indicators – Political stability and absence of Violence / terrorism

WTO : World Trade Organization

# Abbreviations specific for evaluation

AoP: Target producing or purchasing amount of product P ASA<sub>(Mi-Sj</sub>): Available supplying amount of M<sub>i</sub> from S<sub>j</sub>  $C_{Stt_k}$ : Cost of substitute with equivalent of 1 kg of reference material  $M_i$  CD: Cost Difference  $CD_{Stt_k}$ : Cost difference between substitute  $Stt_k$  and reference material  $M_i$ CL : Company location  $Con_{(M_i-F_l)}$ : Contribution of M<sub>i</sub> to the functionality F<sub>1</sub> in the product CR: Contribution Rate  $D_{(M_i)}$ : Demand amount of  $M_i$ EA : Economic Accessibility  $EI_{(M_i)}$ : Economic influence of the i<sup>th</sup> material  $F_{(M_i)}$ : The functionality offered by the i<sup>th</sup> Material

 $F_l$ : The l<sup>th</sup> functionality

 $F_l$ ,  $_l = 1$  to H; Functionality offered by materials to the product. There are H functionalities in total.

FSW : Functionality Satisfaction with Weighting

 $FSW_{(F_l-Stt_k)}$ : Functionality satisfaction with weighting of functionality  $F_l$  of materials  $Stt_k$  $FV_{(M_i)}$ : Functional value of the i<sup>th</sup> material to the product

GF<sub>L</sub>: The L<sup>th</sup> general functionality

 $GF_L$ ,  $_L = 1$  to Z ; General functionality offered by materials for the product. There are Z general functionalities in total.

 $HF_{S_j}$ : Human. Humans are a vital factor in purchasing or business dealings. A reliable and royal partner (human) assures the quality of the relationship between two companies.

 $Inn_{S_i}$ : Innovation. Effort that supplier  $S_j$  makes for innovation. Companies can take

advantage of innovative materials offered by suppliers by becoming more competitive.

 $L_{(S_i)}$ : The j<sup>th</sup> supplier's location (city and country)

LoP: Production loss of product P

M<sub>i</sub> : The i<sup>th</sup> Material's name

 $M_i$  ,  $_i = 1$  to N ; Materials in the candidate pool to be analyzed. There are N materials in total.

 $M2R_{Stt_k}$ : Mass of k<sup>th</sup> substitute needed compared to 1 kg of reference material

 $MV_{(F_l-Stt_k)}$ : Measurement value (MV) of  $F_l$  of substitute  $Stt_k$ 

P: Product name

 $PoM_{Stt_k}$ : Price of material  $Stt_k$  per kg.

 $Price_{(M_i-S_i)}$ : Price of M<sub>i</sub> offered by S<sub>i</sub>

 $QoM_{S_i}$ : Quality of supplying product. Quality of supplied materials from supplier  $S_j$  directly

affects quality of products the company will produce.

 $R_{(M_i)}$ : The i<sup>th</sup> Material's mass ratio in the product

**RDR : Resource Depletion Ratio** 

RDRBR: Resource depletion ratio benchmarking with the reference material

S<sub>j</sub>: The j<sup>th</sup> supplier's name

 $S_j$ , j = 1 to X; Suppliers of materials. There are X suppliers in total.

 $S_{(M_i)}$ : Supplying amount of M<sub>i</sub>

 $Stt_k$ ,  $_k = 1$  to Y; Substitutes. There are maximum Y substitutes of materials.

 $SA_{(M_i-S_i)}$ : Supplying amount (purchasing amount) of  $M_i$  from  $S_j$ 

 $SR_{(S_i-M_i)}$ : Supplying ratio of  $S_j$  for  $M_i$ 

Thh.  $U_{(F_1)}$ : The threshold's unit of  $l^{th}$  function

 $Thh_{F_l}$ : Threshold settled for the functionality  $F_l$ 

 $TIM_{S_j}$ : Timeliness3. Delivery time of  $S_j$ 

TM : Technology Maturity

 $W_{(F_l)}$ : Weighting (Importance) of the functionality  $F_l$  to  $GF_L$  in the product

 $Xch_{S_j}$ : Exchange. An exchange between the company and its supplier  $S_j$  in terms of company strategies, newsletters and perspectives.

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# **CHAPTER 1**

# **INTRODUCTION**

The development of society and technology requires more and more resources and discovers more and more novel uses of materials. Some materials that nobody shows any interest in today may become the favorites of tomorrow. Some products, especially the high-tech ones are more and more complex in terms of structure and materials. At the same time, comparative advantage makes economic activity more optimized i.e. the companies and countries are more specialized on what to produce. For example, a country that contains certain materials may not exploit them but focus on the sectors where it is more competitive. Globalization makes it possible to have access to materials all around the world and also makes one industry or country more dependent on the others than before. Actors involved in the life cycle of one product, including those related to materials, may come from all around the world. Above reasons make supply chain or materials flows of modern products more and more complex. When a malfunction of somewhere in the complex system projects at the level of materials, it leads to problems such as supply disruption, price increase or even a need to reform the system which in return can have big impact on corresponding actors.

Above-mentioned problems are very close to the ones caused by current general understanding of criticality. The term "criticality" or "critical material" is well known thanks to the rare earth crisis in 2010 as well as reports about critical materials issued by the European Commission and the Department of Energy. Materials conflicts are good examples to explain potential influences of criticality of materials and they have occurred at different times and in different countries. For example, a cobalt crisis occurred in the late 1970s due to the civil war in Zaire, which produced the majority of cobalt in the world (Komal, 2015) ; a palladium crisis happened in the 1990s due to export cuts by Russia (Poulizac, 2013) ; a rare earth mineral crisis occurred around 2010 due to export restrictions of China (European Commission, 2010) and the oil shock in 1973 and 1979 occurred due to Arabic countries embargoing supporters of Israel (Sébille-Lopez, 2006). Except for above instances, material crises are the results of interplay among numerous parameters. Zaire was the main producer of cobalt at that moment and the civil war interrupted mining activity as well as rail transport of mined minerals. Even though Zaire managed to produce more cobalt in 1978 than ever before, it was still far from enough compared to the demand of that moment which increased sharply

due to increase of global economy. The price of cobalt increased from 22.5 \$/kg in 1960 to 120 \$/kg in 1980 (1998 normalized price). Substitutes for its usage in ceramics and paints were easily obtained, but not all applications of cobalt could be replaced so easily, as in super alloys for jet engines (Alonso, 2010). Meanwhile, material crises can heavily damage industry and economy. For example, the palladium crisis at the end of the 1990s caused more than \$1 billion in losses to American car manufacturers, as one car contains less than 28 grams of palladium (Poulizac, 2013). During the rare earth crisis in 2010, many high-tech companies were affected as well. Therefore, it is important to know what parameters may influence the criticality of materials and how they affect it, how to determine the criticality and what should be done to prevent or mitigate issues caused by criticality.

To conclude, development of society, globalization and comparative advantages make material crisis more likely to happen in the future and make it more urgent to learn the criticality of materials. Studies of criticality of materials can allow us to have a global view of whether the system to satisfy the related products, sectors or countries is at a good state or not. Furthermore, criticality studies tell us which materials deserve more attention so that industries can take precautionary measures or countermeasures in order to burden lower impacts caused by materials' criticality and have a system more sustainable.

The aim of this Ph.D. study was to understand what criticality of materials is and how to determine it at product level. In more detail, it included following objectives:

- i. Draft an overall map of criticality research area. Learn the progress history of criticality research to see what has been done and what needs to be done in this research area in order to make the thesis well positioned and offer prospective.
- ii. Find parameters which impact the criticality of materials. The objective is to diagnose the phenomenon of criticality in order to find what can make a material critical.
- Define the criticality of materials. Definition implies a proper understanding of the term - criticality. It is a synthetic of what makes a material critical and under which conditions.
- iv. Develop an evaluation methodology / model for the criticality of materials at product level. Write guidelines or methodology which can help us carrying on a critical material study. Develop a quantitative evaluation model which can be used directly to determine the criticality of materials at product level.

This dissertation is structured based on these objectives. A brief summary of each chapter is stated below.

Chapter 1 introduces this dissertation by stating firstly the motivation for / importance of this research topic then related field, followed by the objectives of PhD and finally structures of this dissertation.

Chapter 2 responds to objective (i) and reviews mainly on 48 studies which dated from 1974 to 2014. Review methods were firstly stated. Then review results were stated including the history of criticality, research areas, institutes launched the studies, materials analyzed, materials designated as critical, definitions, evaluation methodologies and data sources of reviewed studies. Finally a diagram concludes criticality research field and shows what needs to be done.

Chapter 3 responds to objectives (ii) and (iii). Firstly research methodology of diagnosis was stated: Based on dictionary of key words like "critical", "strategic" and "important", understandings from review and a scope limitation, a reflection of key criteria of criticality is generated. That leads to an embryonic form of criticality mechanism which is then enforced by criticality indicators appeared in reviewed studies and by a fishbone diagram of criticality causes. Finally a more complete diagram which shows the impact parameters is illustrated, followed by the definition proposed.

Chapter 4 responds to objective (ii) and (iii) as well. It is a comprehensive case study of rare earth materials which serves as a support of criticality diagnosis and an illustration of critical material issue. This chapter firstly introduced rare earth materials in terms of history and properties. Then supply chain or rare earths is analyzed. After that, history of rare earth industry of current production dominating country - China is stated as well as its corresponding policies, followed by recent international attentions to rare earths as well as their price involvement. It ends with reflection of criticality regarding to this rare earth issue.

Chapter 5 responds to objective (iv). This chapter describes the criticality evaluation methodology at product level. It firstly stated the methodology for general scenario and a quantitative evaluation model on basic scenario. Connections between impact parameters and criteria in the basic scenario are also stated. After that, calculation methods of criteria of basic scenario are stated. Finally, it ends with data treatment for results as well as the presentation form.

Chapter 6 contains two applications based on the basic scenario criticality evaluation model stated in the previous chapter. Due to resource limitation and confidentiality, some information is hypothetical. The first illustrative application is about permanent magnet where two materials were evaluated. The second application is about Light Emitting Diode (LED) where 12 materials were evaluated. Both applications contain scenario description, data profiles, criteria calculation, results presentation and sensitivity or completeness analyze.

Chapter 7 is discussions of above chapters, some personal observations and perspectives.

Chapter 8 concludes this thesis by firstly restating research questions with answers, then listing contributions.

# **CHAPTER 2**

# LITERATURE REVIEW OF CRITICAL MATERIALS STUDIES

The objectives of this chapter are (1) to review existing works about critical materials in order to better understand this research domain for following research work; (2) to support other researchers who want to carry on a critical materials study by showing existing definitions of criticality, existing methodologies for determining the critical materials, data sources used in other studies etc.; (3) to determine the research gaps which served as research orientation for this thesis.

The main content of this chapter are published as the article below:

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# 1. Introduction of criticality research activity

The recent rare earth materials debate in the World Trade Organization (WTO) and other materials conflicts stated previously all showed the importance of certain materials to numerous industries and even to the economy, defense and politics of individual countries. This fact drove some authorities to launch organizations which focus on critical materials and conduct studies on them. A good understanding of current or potential future situations of criticality of materials can help stakeholders to make better decisions to mitigate the criticality issues or take measures in advance. Furthermore, a review of critical materials studies provides a global view of this research area and can serve as a reference for future critical material studies. Although there have already been some review papers (Erdmann and Graedel, 2011, Speirs et al., 2013b, APS & MRS, 2011, Lloyd et al. 2012).,this chapter is more comprehensive by covering more studies and offering some unique points like critical / materials coverage, definitions analysis, databases and research gaps.

The structure of this chapter is as follows: Firstly the review methods is introduced; Secondly, the critical research development and results are described, including the history of criticality research activities, the institutes launched the critical materials studies, a collection of materials which have been designated as critical or covered in the examined studies as well as

definitions, evaluation methodologies and data sources used in the reviewed studies; Finally, a global view of this research area is stated as well as the research gaps.

### 2. Materials and methods

The studies reviewed were from scientific databases, governmental or professional reports and websites. The forms of data vary from government bill (Act), book, journal, magazine, report, dissertation and other documents. The referenced journals include "Resources, conservation and recycling", "Resources Policy", "Renewable and Sustainable Energy Reviews", "Environment Science & Technology", "Applied Energy", "Ecological Economics", and "Science of total environment". The magazine taken into account was "Mechanical Engineering Magazine". In terms of reports, the majority were originally issued for the sake of governmental use.

The reviewed studies dated from 1974 to 2014. For this chapter, a total of 48 studies (see supporting information for more information) were considered, of which 48% were conducted by American institutions and researchers, 44% by European institutions researchers, and 6% by other international researchers. Nevertheless, the scope of this literature review is limited to English sources which are publicly accessible, except for two German studies which were cited as Roelich et al. (2011) because of its English summary and one French report (Barreau et al., 2013). For the Japanese study conducted by the National Economic Development Office (NEDO), I only found a presentation form (Shinko research, 2009). Lacking German and Japanese speaking skills, I only checked the supplementary English summary for the German studies and the PowerPoint presentation for the Japanese study. However, from the understanding of their English introductions, those studies should be included in the criticality research area, which is why they were covered as well. The other studies, which were non-English or non-accessible in public, were not covered.

To collect the data, approaches below were applied:

1) Use direct key words to search for corresponding studies. In "Science Direct", "Google", and "Google Scholar", following key words "critical materials", "criticality", and "critique" in French were used to search for the information.

2) First round review: After having searched the key words on research engines and scientific websites, the items which contain above key words or closely related to criticality were collected and examined.

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3) Select the references which are related to critical research area from studies found in the first round. After reading the items collected in previous approach, references cited in those items were also checked. The articles whose titles are related to criticality were then collected.4) Second round review: After the related articles from references being collected, they are reviewed and sorted.

5) Repeat the approach 3) and 4).

6) Use key words to expand the research scope. The key words include: availability, resources strategy (and resource strategies), strategic, material security, resource scarcity, scarcity, dynamic, materials and metals. This approach is to cover the articles which have used different notions than critical but have stated similar information of criticality.

7) Third round review: articles found in the expanded scope were reviewed and sorted. The articles which were closely related to criticality and cited the references in the expanded articles were then examined.

The review approaches were:

1) Based on the three review rounds, collecting the appropriate data (i.e. critical materials studies).

2) Organizing them in an Excel file with the following information: article name, year, institution, geographic location of institution, type of institution, regional scope, phases (to see Figure 3), research scope, highlighted sectors, materials type, development of a criticality assessment methodology or not, proposition of mitigation approaches, geographic area of research, policies, designation of a list of critical materials or not.

3) Tracking the progress and development of criticality research area. In other words, track when the criticality or critical materials studies began and how many studies were conducted each year in order to obtain an overview of this research area.

4) Extracting the scopes and drivers of reviewed studies.

5) Identifying the coverage of materials and sectors. i.e. which materials and sectors drew the attention of researchers and organizations.

6) Extracting the definitions (theoretical core) used in those reviewed studies.

7) For those which developed an evaluation methodology, their basic concepts, principal parameters (dimensions) and indicators which were used to determine the criticality in their studies were extracted.

8) Extracting the materials that have been determined as critical in the reviewed studies.

9) Extracting the data sources used in the reviewed studies.

10) Analyzing above information to find the research gaps in this area, to state the mitigation approaches of criticality and to discuss the observations.

# 3. Critical research development and results

### 3.1 Progress and development of critical material studies

Dating back to Bronze Age, copper was used to make weapons and farming tools. Before smelt and cast iron technology was discovered, copper was important and faced shortage problem in some countries once a while. Later around 300 A.D., Roman Emperor had issued the embargo of the following "strategic commodities" due to shortage and their importance to the empire: cereals, iron, copper, horse etc. (Stavrianos, 1999/2006). These phenomena are similar to current criticality events. Now days, the products are more and more complex which need more and more indispensable worldwide materials. This fact made the criticality an impending topic to work on. In spite of that, the official notion of criticality appeared firstly in the end of 20th century (The white house, 1974) and the evaluation methodology was firstly developed by the National Research Council (NRC) (2008) among the examined studies. Not until the rare earth conflict in 2010, the criticality issue started drawing more and more attention. To sum up, the criticality research is increasingly studied recently even the idea of criticality is not new.

One of the first document closely related to critical materials appeared in 1974 (The White House, 1974). It was a governmental memorandum about critical imported non-fuel commodities. Since commodities cannot be separated from materials, and the policy options taken for both of them are similar, it is taken account in this review. 34 years later, the first direct critical materials study (National Research Council, 2008) built a "criticality matrix" to determine critical minerals from a list of candidates. The cited drivers of conducting an assessment of materials, social or environmental pressure, policy measures and concentration of production (Lloyd et al., 2012).

For now, there is no agreed definition (Lloyd et al., 2012) of criticality or assessment methodologies. Some works, such as the studies of availability, scarcity, supply risks etc., were closely related to criticality, for instance, the materials efficiency study conducted by Söderholm and Tilton (2012). According to the reviewed studies, availability is one important parameter which influences the criticality of the materials. Notwithstanding that the

availability cannot fully represent the criticality, it can still offer useful information related to the potential criticality assessment. Some studies were only focused on the aspect of availability for certain materials. For example, the availability of indium and tellurium relating to thin film photovoltaic (PV) technologies was studied by Candelise, Speirs and Gross (2011). The world production data, reserve data, market dynamic and prices of these two materials were analyzed in their work. Cleveland (1993) stated an alternative measure of natural resource scarcity for petroleum resources. His study combined a new biophysical index with traditional economic indicators, which include market price, unit cost of extraction and average total cost of extraction of natural resource. This measure's coverage is close to the current critical assessment. Some authors also used the notions "critical", "strategic" or "scarce" interchangeably in their studies. As we can see here, researchers have already been working on sub aspects of "criticality" without having an overall concept of criticality. This is why these studies with similar notions of criticality were added to the review list.



3.2 Institutions and geographic locations of the reviewed studies

Figure 1: Geographic distribution of reviewed critical materials studies

Among the reviewed studies, half of them were conducted in the United States (as shown in Figure 1). The majority of the remaining studies were conducted in Europe (mainly the UK, the Netherlands and Germany). One study was conducted in Japan. All of them were

developed countries and more dependent on import materials for manufacturing high-tech products. They are among the countries that launched a rare earth case against China in the World Trade Organization (WTO, 2015). More than half were conducted by research institutes and universities and one third was governmental institutes. The rest of reports were released by other research bodies like consulting companies, non-profit research organizations and associations. Hence, most of their studies were related to government by obtaining governmental funding, carrying out projects for government, providing information for government and so on. In reality, governments have been currently driven this research area. Some industries have conducted their own studies on criticality, such as General Electric (Duclos, et al., 2010) and Tesla (DeBord, 2015), however, due to the confidentiality, details of how they drew their conclusion of criticality were not available to the general public.

# 3.3 Materials covered and designated critical

Some studies designated directly certain materials as critical ones without comparing to others. For example, Hatch (2011), Rademaker et al. (2013), and Massari & Ruberti (2013) regarded rare earth materials as critical by default and then focused on situations or strategies of those materials' supply and demand. Table 1 shows the categories, as well as detailed names of materials covered by existing studies. The majority (40 elements) of materials which were analyzed in reviewed studies were metals. When two different materials contain the same element, they were only counted once in this chapter. To highlight the importance of platinum group metals (PGM) and Rare Earths (RE), these two metal groups' elements were counted separately from other metals.

The current studies on critical materials did not only cover metals. Some non-metallic elements, metalloids, compounds and organic resources have also been studied (see Table 1). For example, graphite, fluorine, nitrogen, phosphorus, selenium, bromine, wood etc. were studied. All the groups in the periodic table are covered. Elements like gallium, indium, cobalt, tellurium, germanium, niobium and the rare earth group were the most frequently covered within the 32 studies. Even some materials which are widely found in the Earth's crust were included, for instance, silicon. Several mass produced metals, for instance copper (Nassar et al., 2011) and iron including its principal alloying elements (Nuss et al., 2014) were also analyzed for their criticality. However, copper was identified as not critical for the general American economy in the National Research Council's report (NRC) (2008). This fact highlights the point of view stated by the NRC (2008) or the European Commission (EC)

(2014) that materials which were not designated as critical in their studies were still important and might be critical for other organizations or industries. In general, a critical materials study selects the candidate materials which represent partly the scope of that study. These candidates consist of materials needing further assessment by experts or professional committee members. For example, a national-level study should range from the materials required massively in major economic activities to those whose consumption is small but important for some emerging technologies.

Table 1 : Categories and details of materials covered by current critical materials studies ("cover" involves the materials which have been analysed regardless of being determined critical or not)

Materials	Number of	Details of materials	
category	studies		
Metal	40	aluminum, barium, beryllium, bismuth, cadmium, calcium, cesium,	
		chromium, cobalt, copper, gallium, germanium, gold, hafnium,	
		holmium, indium, iron, lead, lithium, lutetium, magnesium, manganese,	
		mercury, molybdenum, nickel, niobium, potassium, rhenium, rubidium,	
		silver, sodium, strontium, tantalum, thallium, tin, titanium, tungsten,	
		vanadium, zinc, zirconium	
Non-metal	12	ammonia, arsenic, borates, boron, bromine, diamonds, graphite, helium,	
		iodine, phosphate, phosphorus, selenium	
Actinide	1	uranium	
Alloy	3	beryllium copper master alloy, chromium ferro, manganese ferro	
Compound	2	silicon carbide, sodium carbonate	
Metalloid	3	antinomy, silicium, tellurium	
Organic	4	coking coal, pulpwood, natural rubber, swan softwood	
resources			
Unsorted	14	chromite, clays (kaolin), diatomite, feldspar, fluorspar, gypsum,	
minerals		limestone, mica, perlite, potash, quartz crystals, silica sand, talc,	
		vermiculite	
Platinum	6 + platinum	11 (58%) studies studied platinum group without distinguishing	
Group	group	individual elements	
Metals			
Rare Earth	17 + rare	15 (60%) studies studied rare earth group without distinguishing	
Elements	earth group	individual elements	
Total	80 materials +	- Rare Earth Elements (REE) + Platinum Group Metals (PGM)	

Groups	Critical materials (from the most often designated critical to least)	<b>References (studies which gave a list of critical materials)</b>
Group 1: Clean technologies requirements	In, Nd, Ga, Dy, Te, Ge, Y, Co, RE group, Eu, Tb, Li, Se, Ag, Cd, PM group, Ta, Sb, Pt, Sn, Be, Cu, CaF2, Graphite, Mg, Mo, Pd, Ru, La, Ce, Pr, W, Al, As, Cr, Au, Hf, He, I, Fe, Ni, Pm, Sm, Gd, Ho, Er, Tm, Yb, Lu, Sc, Si, Ti, V, Zn	(Department of Energy, 2010), (Department of Energy, 2011a), (Moss et al., 2011), (Goe and Gaustad, 2014), (APS & MRS, 2010), (Speirs et al., 2012), (Speirs et al., 2011), (Candelise et al., 2011b), (Speirs et al., 2013a), (Smith et al., 2012), (Rademaker et al., 2013), (Öko- Institut e.V., 2009), (Bachér et al., 2013), (Resnick Institute, 2011), (Angerer, 2009)
Group 2: National security requirements	Al, Cr, Mn, Sb, Be, Bi, CaF2, Ga, Ge, Y, SiC, Ta, Sn, W, Co, Nb, Tb, Dy, Er, Tm, Sc, chromium-ferro, Cu, Pb, Hg, PM group, Rh, Ru, Re, natural rubber, Sr, Zn	(OUSDATL, 2013), (Thomason et al., 2010), (Congressional Budget Office, 1983)
Group 3: General economy requirements	Mg, In, Nb, Al, Sb, Co, Ga, RE group, PM group, W, CaF2, Ge, Graphite, Li, Mn, Be, Cr, Re, Ta, V, Ba, Borates, Cu, Au, Mo, Pt, Si, Ag, Ti, Zn, Feldspar, Fe, Pb, Hg, Perlite, Sr, Talc, Sn, Ammonia, As, Bi, B, Br, Cd, Clays (kaolin), Coking coal, Diatomite, Gypsum, Ho, Limestone, Lu, Nickel, Phosphate, P, Ir, Os, Pd, Rh, Potash, Eu, Gd, Tb, Se, Silica sand, Soda ash, Te, U, Vermiculite, Zr	(European Commission, 2010), (National Research Council, 2008), (European Commission, 2014), (Morley and Eatherley, 2008), (Silberglitt et al., 2013), (Statistics Netherlands, 2010), (Barreau et al., 2013), (Parthemore, 2011), (Congressional Budget Office, 1983)

Table 2: Materials designated or determined as critical in accordance with sectors and regions

As shown in Table 2, materials which were determined or designated critical in the reviewed studies were sorted into three groups. Group 1 relates to application in clean technology which involved permanent magnets, advanced batteries, thin-film semiconductors, phosphors, wind turbines, electric vehicles, photovoltaic, energy-efficient lighting etc. Indium (In) was the most mentioned element for these technologies. Other significant elements include Neodymium (Nd), Gallium (Ga), Dysprosium (Dy), etc. in decreasing order. Group 2 contains the materials which were often designated critical for satisfying national security requirements (the materials needed to secure the basic operations and safety of a country), for example national defense, essential civil usage or national emergency situations (an emergency related to national defense). Aluminum (Al) was the most mentioned element for this group, followed by Cr (Chromium), Mn (Manganese), Sb (Antimony) and so on. Main constituents of the second group are high demand materials and only a few are low demand materials like Dy, Y, etc. In this group, one non-metallic material (natural rubber) was designated as critical. Group 3 involves general industrial activities that influence the country's economy and geographically limited in a country or administrative area. Mg

(Magnesium) was the most often critical designated in terms of general economy, followed by In, Nb, Al, Sb, and so on. This group also contains non-metal materials like graphite, clays and phosphorus. The constituents of this group's critical material list are more varied than other two groups. The objective of Table 2 is to help researchers reduce the scope while deciding materials candidates for their studies by showing the list of which were more often designated as critical in terms of different sectors.

#### 3.4 Definitions of criticality or critical material from the studies

Currently there are several definitions for critical materials, but none was accepted worldwide. In Table 3, eight versions of definitions that found in the reviewed studies were assembled. The extracted keywords are very similar to the dimensions for evaluating the criticality (to see Table 4). Supply (risk or restriction) is the one mentioned in all definitions. Some definitions have illustrated the scope, for instance, the national emergency situation (96th Congress, 1979), clean energy (DOE, 2010), novel technologies (APS & MRS, 2011) and raw materials (EC, 2010). Among all the reviewed studies, the organizations from the same region are more likely to agree to the same definition. For example, the Statistics Netherlands (2010) and the France General Office of Strategy and Forecasting (in French: France Commissariat Général à la Stratégie et à la prospective) (Barreau et al., 2013) in Europe applied the definition of the EC. Massari et Ruberti (2012) and Rademaker et al. (2013) also agreed with the EC's definition and analyzed rare earth elements deeper as critical raw materials. In terms of the United States, the criticality evaluation studies in Yale University are more agree to the National Research Council (NRC)'s definition only by adding the environmental aspect. However, the definition proposed by the DOE is more similar to the second version proposed by the EC. Among reviewed studies, the EC definition is more widely accepted. Despite different versions and there is no consensus of definition yet, we might do the selection according to the context or scope of own study. If we want to conduct a critical materials study for a country or an area, we might apply the definition proposed by the EC, the DOE or the NRC. If the country is under a state of war preparation or conflict, we might apply the 96<sup>th</sup> Congress definition. If we want to analyze one material's market, we might apply the Poulizac's (2013) definition. Also if we focus more on technology, we might apply the APS & MRS, Goe, M. et al and Roelich, K et al. by combining with supply chain risk management. Table 3: Definitions of criticality or critical materials in the reviewed studies (\* note: key words in Italics are related to context of the definition)

Reference	Definitions	Key words or dimensions*
96th	The term "strategic and critical materials" means materials that (A) would be needed to supply the military, industrial, and	Supply
congress,	essential civilian needs of the United States during a national emergency, and (B) are not found or produced in the United	Demand
1979	States in sufficient quantities to meet such need	National emergency
National	A material can be regarded as critical only if it performs an essential function for which few or no satisfactory substitutes	Function
Research	exist, in addition, an assessment also indicates high probability that the supply of the material may become restricted,	Substitution
Council,	leading either to physical unavailability or significantly higher prices for that material in key applications.	Supply restriction
2008		Unavailability or High price
EC, 2010	To qualify as critical, a raw material must face high risks with regard to access to it, i.e. high supply risks or high	Supply risk
	environmental risks, and be of high economic importance. (version 1)	Environmental risk
	Critical raw materials are those which display a particularly high risk of supply shortage in the next 10 years and which are	Importance
	particularly important for the value chain (version 2)	
DOE 2010	<i>Criticality is a measure that combines importance to the clean energy economy and risk of supply disruption.</i>	Supply risk
		Importance (clean energy)
APS & MRS,	If a new technology that employs a rare element were to be widely deployed, widely enough to make a significant	Energy
2011	contribution to our energy needs, quantities of the rare element might be required that exceed present production, perhaps	Novel technology emerging
	by orders of magnitude. We shall refer to such an element as (potentially) an energy-critical element (ECE). (version 1)	Demand
	"Energy-critical element" (ECE) is a class of chemical elements which are critical to energy related technologies. In this	Production (equivalent to
Deulines 5	aefinition, the ECEs are limited into those with novel uses. (version 2)	supply)
Poulizac, F.,	criticality is the consequence of a confidence of factors: (a) market imperjections in either materials production or consumption, or both: (b) the influence of non-primary market actors on the market, such as appearaments and invectors:	Non primary market actors
2015	(c) the fragility of the resource supply chain to "common mode" disruptions arising from operating dislocations, either	Supply discuption
	(c) the fragmity of the resource supply chain to common mode ansarptions ansing from operating dislocations, either stochastic (e.g., natural disasters) organizational (e.g., labor unrest) or institutional (e.g., non-competitive behavior of	Substitution
	firms such as cartelization): and (d) a relatively sparse set of feasible — or at least not cost prohibitive — alternative	Function
	technologies to achieve comparable functionality using different materials	Tunction .
Goe, M. et	Material criticality, as defined here, is a relative concept in that it compares materials against each other to determine	Relative
al., 2014	which materials have the areatest risks of disruption to supply.	Supply disruption risk
Roelich. K et	We define criticality as the combination of the potential for supply disruption and the exposure of pre-determined	Supply disruption
al., 2014	pathways (or scenarios) of technology roll out to that disruption	Impact to technologies

# 3.5 Analysis of criticality evaluation methodologies applied in the reviewed studies

#### Basic concepts and dimensions of methodologies applied in the reviewed studies

Figure 2 shows four basic concepts extracted from reviewed studies: (a) the two-dimension Cartesian coordinate system, (b) the three circles model, (c) the three-dimension Cartesian coordinate system, (d) the five-dimension radar chart. The first criticality evaluation methodology, whose basic concept is named as criticality matrix (see Figure 2-a), was developed by the NRC (2008) of the U.S. This concept has two dimensions. It includes material's importance in use (impact of supply restriction) as the vertical axis and material's availability (supply risk) as the horizontal axis. It became the cornerstone for similar subsequent studies and was adopted by most other critical materials studies, such as the EC and the DOE. In 2011, another concept, containing three dimensions was developed (Graedel et al., 2011) for metal criticality determination (to see Figure 2-c). It contained supply risk, vulnerability to supply restriction and environmental implications. The environmental dimension had already been considered, but separately, in the EU (European Commission, 2010) study where it was based on the two-dimension concept developed by the NRC. The above two basic concepts are the most recognized ones. In 2009, Öko-Institut (2009) conducted three-prioritization for assessing critical metals (to see Figure 2-b) which considered the supply, demand and recycling restrictions. In 2013, M:5 was developed by Claire Marie Poulizac (Poulizac, 2013) for assessing the criticality of minerals. Compared to others, this one is more industrial specialized. The M:5 model considered the following dimensions: physical constraints, institutional inefficiencies, sustainability impacts, relative importance of the industry and importance to the company. There are other variations which considered different dimensions. The integration of which dimensions were chosen by different studies was presented in Table 4. From Table 4, we can see that, for the majority of studies, supply was considered as a principal parameter (dimension) influencing the criticality of materials, only with one exception (Bachér et al., 2013). Demand and environmental factors are the next in importance in those studies. Parameters like 'vulnerability to supply or supply restriction', 'economic', and 'importance or impact' were also considered in certain evaluations. A few studies considered 'recycling', 'material' or 'innovation' as major parameters for evaluating criticality. Criticality is also influenced by several dynamic aspects, for instance, price and supply oscillations affect the demand (Poulizac, 2013). Knoeri et al.

(2013) stated that the dynamic aspect should be included in the critical determination by combining an agent-based model and materials flow analysis.



Figure 2 : Basic concepts used in current criticality assessment

Keywords	Demand	Supply	Vulnerability to supply restriction	Environmental	Importance or impact (included economic aspect)	Recycling	Materials	Innovation
Other statement forms Studies	Demand risk/growth ; Total annual purchase ; Raw materials demand of a specific application	Availability ; Supply risk ; Supply disruption potential ; Supply and price risk	Exposure to supply disruption	Environmental Implications; Environmental country risk	Importance in use or impact of supply restriction ; Importance (to clean energy) ; Impact of an element restriction on the company; Economic importance	Recycling restriction	Material risk	Innovation
National Research Council 2008, Department of Energy 2011a		1			1			
Department of Energy 2011a, Department of Energy 2011a								
Morley and Eatherley 2008		1					1	
Poulizac 2013, OUSDATL 2013	1	1						
Roelich et al. 2014		1	1					
Nuss et al. 2014, Graedel et al. 2012, Nassar et al. 2011		1	1	1				
European Commission 2010, Goe and Gaustad 2014,European Commission 2014		J		1	1			
Öko-Institut e.V. 2009	1	1				1		
Duclos, Otto, and Konitzer 2010	1	1			$\checkmark$			
Bachér et al. 2013				1	✓			1

#### Analysis of databases used in the reviewed studies

The reviewed studies obtained data from following sources: open or private databases; reports or articles; advice from experts by interviews, meetings, surveys or workshops; requests for information (RFI) from capable affiliated institutions or consulting agencies.

Among them, public databases are the first choice of most authors. For example, data from the United States Geological Survey (USGS) and the World Bank are widely used in the reviewed studies. Several data sources have geographic limitations. For example, the Chemical Society of France (in French: Société Chimique de France) (SCF) and the National Institute of Statistics and Economic Studies (in French: Institut National de la Statistique et des Etudes Economiques) (INSEE) are both French institutions whose research is usually related to France. Consulting agencies may offer useful information to researchers doing critical materials studies, however, the cost of data is then a significant factor. For example, Eco-invent is a pay-for-use database widely used for the Life Cycle Inventory (LCI) and the Life Cycle Impact Assessment (LCIA) data. Several institutes, such as the Critical Material Institute (CMI), may only respond to related governmental organizations. Besides the open data sources listed in Table 5, other sources such as industries' annual reports, conferences, forums or correspondent associations may also provide information. The NRC (2008) listed American and international data sources for mineral information.

# Table 5 : Part a. Databases and examples of data that can be found with open access

Database	Database institute	Data type	Data examples available
Mineral commodity summaries Mineral yearbook Mineral industry surveys (monthly)	United States Geological Survey (USGS)	Geography	Mine production (global and by country) Reserve amount (global and by country) Resource amount (global and by country) Import, export and consumption amount (U.S.) Price (U.S.)
World Economic Outlook Database Global Financial Stability Report IMF Data Mapper SDRs per Currency Unit	International Monetary Fund (IMF)	Economy	Capital account, Commodity price, Current account Economic growth rate, Exports, Final statistics Foreign direct investments, Gold, GDP, GNI, Imports Oil price, Reserves, Trade
Trade statistics	International Trade Administration (ITA)	Economy	National U.S. Trade Sub-national U.S. Trade U.S. Exporting companies Jobs supported by exports
International Economic review Industry trade and technology review	International Trade Commission (ITC)	Economy	U.S. Trade development International Economic comparisons Statistical Tables Factors which affect U.S. manufacturing
International Trade Statistics Database	UN Comtrade	Economy	Total merchandise trade (by country) Total services trade (by country) Imports, Exports Global trade data (monthly and annual)
Energy balance flows Energy indicators European gas trade flows Key World Energy Statistics	International Energy Agency (IEA)	Energy	Coal, Energy balance CO <sub>2</sub> emissions from fuel combustion Energy production (by country), Oil
Table 5. Part b. Databases and examples of data that can be found with open access

Database	Database institute	Data type	Data examples available
Fund of peace	Fund of peace	Human right, stability, policies	Fragile States Index (by country)
Eurostat database	Eurostat	Interdisciplinary, international data	International trade Statistics on industrial production and international trade
World bank databases	The World Bank	Interdisciplinary, international data (health, social, environmental, financial, technology etc.)	GDP, GNI, Total reserve, Labor force, Energy imports Import value index, Exports of goods and services World Governance Indicator
AZoM (industrial website)	A to Z of materials Science	Materials	Suppliers, Applications, Industries, Metal stores
World mining data	World Mining Congress	Mining data	Total minerals production by country World production of Iron and Ferro-alloy Metals World production of Non-ferrous metals World production of Precious Metals World production of Industrial minerals World production of Mineral fuels
Industrial Minerals Data	Industrial Minerals	Latest news Price Market brief	Graphite, Fluorspar, Alumina/Bauxite, Frac Sand, Lithium, Magnesia, Rare earths, Soda ash, Zircon etc.

## 4. Overview of criticality research domain and future research possibilities

In general, when we carry out a critical materials study, our thinking follows the right-to-left red flashes in Figure 3. At first, we determine the final goal which is to find solutions to mitigate criticality issues or to prevent certain problems in the future. In order to arrive at the final goal, an evaluation model is needed to determine which materials are critical and how they are critical. To achieve that, a diagnosis of which parameters influence criticality and how they affect it is required. According to the above backward thinking to obtain the final goal, a three-phase logical order of execution is established (to see the left-to-right yellow flashes in Figure 3). The first phase in the criticality research field is to conduct a comprehensive study of all the parameters which influence criticality and to learn the mechanism of criticality. It can be considered as a pre-phase or a diagnosis of criticality. The next phase is to determine the criticality of materials with an evaluation methodology. Then the third is to find mitigation approaches for criticality issues, to prevent the problems in the future. However, that is not the order that reviewed studies followed. Most of them were about determination, either quantitatively or qualitatively, of critical materials. There are studies which evaluated the critical materials for a specific area, e.g. by the European Commission (2010). It determined 14 critical materials for Europe in 2010, and was updated last year (European Commission, 2014). Some studies focused on particular technologies, e.g. the DOE (2011b) of the U.S. They evaluated critical metals for clean energy. Some studies are for certain types of materials, e.g. the criticality of copper family (Graedel et al., 2012) and fours nuclear energy metals (Harper et al., 2015) were analyzed by Yale University. These correspond to the second phase. Some focused on further studies (mitigation / prevention) which were based on the results of the second phase. They were corresponding to the third phase. For example, Statistics Netherlands (2010) analyzed the influence of materials which were determined as critical to Dutch industries by the European Commission. Rademaker et al (2013) focused on one mitigation approach "strategy" for the criticality of rare earth elements (REE). In fact, phase 1 is a potential research area which needs more work. Even if most studies stated briefly the geopolitical, economic and other aspects of criticality, none of them conducted a comprehensive analysis at how those factors may influence the criticality. However, without the diagnostic phase, we cannot prescribe (determine or treat) the "criticality" symptoms properly.

Based on this review, following research gaps have been identified: the diagnosis of impact parameters of criticality, models to evaluate the criticality of materials at product level and building links between different phases. In terms of the evaluation model for a product or the sector of one typical product, the industries might have already developed their own methodology or have other similar tools. Due to confidentiality, that information is not available to the public. That is why I still considered it as an area of work where hasn't been started. In addition, some of the current assessments lack of transparency and information of how they obtained their results. And that also makes those assessments impossible to be reproduced (Lloyd, Lee, Clifton, Elghali, & France, 2012).



Figure 3 : Diagram of the criticality research field.

Note: The light yellow flash (in the top of figure) showed the logical order of execution the research of criticality. The blue flash showed the equivalent blocks in accordance of each phase. The dark orange flash from right to left (in the middle of the figure) showed the backward thinking to obtain a goal. The blue block showed the work area where have been started. The white blocks with blue dotted lines mean the work area where I did not find much information. The blue dotted flashed mean the links between different work areas have not been conducted yet.

## **CHAPTER 3**

# PRE-PHASE (DIAGNOSTIC) OF CRITICALITY

This chapter is about analyzing parameters which influence the criticality of materials (which is called impact parameters) at product level. It is a necessary phase before the development of criticality evaluation methodology according to the previous chapter. This part is named as the "diagnosis of criticality".

## 1. Research methodology of criticality diagnosis

Research methodology to conduct the diagnosis is as below (see Figure 4). 1) Search for key information of "critical", "strategic", and "important" from dictionaries and scientific publications. 2) Review on existing critical materials studies. 3) Ask question "which parameters can influence the criticality of materials at product level?" 4) Reflect on the information of the three previous steps and find key criteria of criticality. 5) Establish the embryonic form of how criticality is influenced (schematic diagram of criticality mechanism). 6) Look into the quantitative and qualitative indicators used in the existing studies to see if they can be added into the embryonic form of previous step. 7) Brainstorming of parameters in the technological, social, economy, political, geographical, and environmental aspects to reinforce the embryonic form. 8) Establish the mechanism of impact parameters of criticality. The obtained impact parameters from the diagnosis part are as showed in Figure 8. At the end, rare earth material is used as case study to check the conformity of the criticality mechanism.



Figure 4 : Research methodology of criticality mechanism – the diagnostic

# 1.1 "Critical", "Strategic" and "Important" key definitions

The key information of "critical" from on-line dictionary is as below ('critical', n.d.): "

- Judge severely and find fault;
- Forming or having the nature of a turning point, crucial or decisive;
- Indispensable, essential;
- Being in or verging on a state of crisis or emergency (mathematics) of or relating to a point at which a curve has a horizontal tangent lines, as a maximum or minimum;
- (chemistry & physics) A value of measurement at which an abrupt change in a quality, property or state occurs urgently needed;
- (medicine) So seriously ill or injured to be in danger or dying;
- (general physics) Denoting or concerned with a state in which the properties of a system undergo on abrupt change of decisive importance;

- (of a patient's condition) Having unstable and abnormal vital signs and one or more unfavorable indicators;"

The key information of "strategic" from on-line dictionary is as below ('strategic', n.d.):"

- *Of, relating to, or characteristic of strategy;*
- Important or essential in relation to a plan of action;
- Essential to the effective conduct of war;
- Highly important to an intended objective;
- Intended to destroy the military potential of an enemy"

The key information of "important" from on-line dictionary is as below ('important', n.d.):"

- Strongly affecting the course of events or the nature of things, significant;
- Having or suggesting a consciousness of high position or authority; authoritative;
- Of great significance or value, outstanding;
- Of social significance, notable, esteemed;
- *Especially relevant or of great concern, value highly;*
- Of considerable distinction;"

#### 1.2 Understandings based on reviewed document

This step is to integrate what I have learned from examined studies into determining mechanism of criticality. For example, how critical material or criticality was defined or interpreted in other studies; which aspects were concerned when they determine or evaluate the criticality of those materials; what indicators were used for evaluation etc. The review offered me answers of above questions and helped me better learn the mechanism of criticality.

#### 1.3 Questioning what materials are critical for the product to a company

First of all, we need to figure out the relation between a material and a product. When a material is demanded by a product, actually it is because one or several properties of this material offer the specific functions that the product required. This theory can also explain the substitution. When another material offers the same function which is required by the product, that material can be a potential substitute. A material contains usually more than one property which relates to more than one use. It means the material can be demanded for different

properties in different products. Therefore, it is easier to analyze the criticality of one material when the scope is limited to a specific functionality. That is also what is interested by a specific industry when they carry on a critical material analysis.



Figure 5 : The relations between a material's properties and a product's functions

For example, gold used as a material for electrical wire is because that its property (conductivity) can offer the function (conduct the electrons without too much loss) required for the product. Silver which has a better conductivity can substitute gold in this function. To sum up, it is the material which can offer a proper conductivity that the product needs instead of a material which is called gold or silver or others properties rather than conductivity that gold or silver has.

Inspired by meanings of "critical", "strategic", and " important" from the dictionary, I searched for the potential answers of the following question in the point of view of a company or an industry: In which situations, one material is critical to product or sector?

Here are answers of possible situations:

- 1) Without the material, a product won't work. The properties offered by the material are indispensable to the functionality required by the product.
- 2) Without the material, the performance of the product will decrease.
- 3) The function offered by this material is needed and indispensable; however this material should not be used in a certain time due to some reasons.
- 4) Getting this material hams the benefits of the company or even makes the company in danger (from social, environmental, regulative pressures etc.).
- 5) Not be able to or difficult to get the functions or properties offered by the material.
- 6) Abrupt changes that the company does not have enough time or resource to adapt to.
- 7) Turning point that affects the company's affaires.
- 8) Make company be a state of crisis or emergency.
- 9) Urgently needed by the world which reduces the access of the company or urgent need by the company that not enough access is available.

# **1.4 Reflect**

This step involves arrangement, filtration and induction of information collected above. At the beginning, the information is arranged according to the categories of their contents. Then I selected the elements which influence the criticality. At the end, it is to think about the interrelations of these elements and group them under different dimensions.

# 1.5 Establish the embryonic form of criticality mechanism



Figure 6 : Embryonic form of mechanism of criticality of material to a product

The figure above is the embryonic form of the criticality mechanism with four dimensions. It is a visualization of previous step - reflection. More explanations are available in the section 2 of this chapter and the complete form is showed in Figure 8.

# **1.6 Look into the quantitative and qualitative indicators in reviewed** studies

Except the contents stated in the previous chapter, here are the indicators mentioned in the reviewed studies.

Table 6 : Indicators appeared in reviewed studies divid	led into group Supply, Vulnerability to supply restriction, Demand
and Environment.	
Group 1 : Supply	Worldwide governance index (WGI)

Group 1 : Supply	Worldwide governance index (WGI)	
Country's Import dependence (%)/Net import	Share of material consumption in a sector	
reliance		
World reserve/production ratio (R/P)	Substitutability of material in a sector	
World byproduct production as % of total world	Recycling rate	
primary production		
Country secondary production from old scrap as %	Hirfindahl-hirshmann index (HHI) of primary	
of Country apparent consumption	material and ore producers	
Domestic production, capacity and ramp-up	Recycling rate	
Foreign production, capacity and ramp-up	Political instability in major supplying	
	region/country	
Secondary domestic supply	Monopoly supply	

Supply from combat adversaries (enemy	Vulnerability of major supplying region/country to	
compatants)	the effects of climate change	
Supply from unwilling countries	countries	
Foreign infrastructure/availability reliability factors	Dependence on virgin resources (lack of recycling)	
War damage factors	Potential to displace virgin material by resource	
	efficiency strategies (potential to increase	
	recycling. re-use, durability, minimization)	
Shipping loss factors	Production-requirement imbalance	
Domestic share of foreign suppliers ("market share")	Companion fraction (YC)	
Usability of supply to satisfy defense demand	Access (YH)	
(market dominators)		
Regional concentration of mining	Environmental constraints (YE)	
Physical scarcity	Abundance in Earth's crust	
Temporary scarcity	Sourcing and geopolitical risk	
Structural or technical scarcity	Co-production risk	
Depletion time (DT)	Demand risk	
Companion metal fraction (CF)	Historic price volatility	
Policy potential index (PPI)	Market substitutability	
Human development index (HDI)	Regional concentration of mining	
Worldwide governance indicators-political stability	Physical scarcity	
and absence of violence/terrorism (WGI-PV)		
Global supply concentration (GSC)	Temporary scarcity	
Share of the country in the world production	Structural or technical scarcity	
Group 2 : Vulnerability to supply restriction	Substitute performance	
Material assets (MA)	Substitute availability	
Substitute performance (SP)	Environmental impact ratio	
Substitute availability (SA)	Price ratio	
Environmental impact ratio (ER)	Corporate innovation	
National economic importance (NE)	National economic importance	
Net import reliance ratio (IRR)	Percentage of population utilizing	
Global innovation index (GII)	Net import reliance	
Percent of revenue impacted	Goal sensitivity (Sc)	
Ability to pass-through cost increases	Price sensitivity (Sp)	
Importance to corporate strategy	Percentage of population utilizing	
Group 3 : Demand	Annual value (Ve)	
Moderate demand growth: > 20% increase of total	Rapid demand growth: > 50% increase of total	
demand until 2020	demand until 2020	
% Country consumption in existing uses for which	Influence of economic changes between the	
substitution is difficult or impossible	reference year and the projected target of year	

Importance of growth in emerging uses that could	Average annual growth rate of activity (production)	
overwhelm existing global production capacity	between the reference year and the time horizon	
Activity rate (production amount) of the	Specific raw material demand of the application	
application (units/a)	(t/unit)	
Defense demand	Relative change in raw material demand due to	
	technological change	
Essential civilian demand	Economic growth	
Imports and Exports	Country's consumption (millions \$)	
Homeland recovery		
Group 4 : Environmental	Share of material consumption in a sector	
Impact on European policies in case of supply	Substitutability of material in a sector	
disruption		
Share of the country in the world production	Recycling rate	
Environmental performance index	Relative Primary embodied energy (Fe=1)	
Energy savings		

The indicators were arranged in four groups above: Supply, Vulnerability to supply restriction, Demand and Environment. In order to present the different ways of expressions, those expressions which may indicate the same or similar meaning were not eliminated.

Supplementary notes are as below. Cleveland (1993) listed the general index used for petroleum resources, for instance, unit cost, relative price, average total cost, yield-per-effort, production growth cycles, field size distribution, energy return on investment, undiscovered resources and average cost of drilling a well. Price is one of the indicators which reflect the economic importance of the material and the scarcity. However its volatility decreases the credibility as being an indicator (Alonso, Field, Gregory, & Kirchain, 2007). Some financial models which are served as decision-making support tools by industries can be used as indicators of criticality as well. Claire Marie Poulizac (2013) mentioned economic abstraction based analytical modelling, financial-based modelling approaches and system dynamics modelling in their critical materials study.

## 1.7 Cause and effect diagram with different aspects

After previous six steps, I used the fishbone diagram (Figure 7) to check the cause of criticality under technological, social, geographic, economic, politic and environmental aspects. The objective of this part is to search for the cause of criticality in another angle in order to have a more complete understanding of criticality.



Figure 7 : Criticality examination under different aspects with the use of fish-bone diagram

## 2. Results of criticality diagnosis

As shown in Figure 8, four dimensions were determined to illustrate the mechanism of criticality of materials at product level: imbalance between demand and supply, accessibility to supply, importance and dynamic factors. These dimensions were decomposed into more detailed levels. The ending of each dimension was named as "impact parameter" of criticality.

#### 2.1 Importance of materials

This dimension represents the importance of materials to the product and consists of functionality, substitutability and economic influence. The functionalities of all the materials comprise the performance of corresponding product. Thus, we require the functionalities offered by the materials instead of the materials themselves (Poulizac, 2013). It embodies the meaning of one material for a product. At the same time, functionality can be obtained from other materials with an acceptable price, a mature production technology and sufficient supply. More often a material can be replaced, less important it is. Finally, economic influence is considered according to cost of each material. Rare earth elements' application as catalysts in petroleum refining is a good example. The price of rare earth materials has increased in 2010. However, rare-earth catalysts were still being used even though catalysts containing zero rare earth elements were already available for petroleum refining. This can be explained by the fact that the prices of rare earth materials influenced barely the final cost of petroleum due to low content of rare earth materials in refining production (Department of Energy, 2010). Impact parameters of this dimension can be confirmed by this case: functionality (rare earth elements' properties as catalysts), substitutability (zero rare earth catalysts are available) and economic influence (increase in rare earth prices had small effect on final cost of refining).

## 2.2 Accessibility to supply

This dimension was divided into two parts. The first part is about the supply that should not be accessed. It concerns accessibility that is restricted due to environmental, legislative or other reasons. For example, mercury is limited to 5 mg for compact fluorescent lamps according to Directive 2002/95/EC. Uses of other materials such as lead, cadmium, or hexavalent chromium are also limited (European Commission, 2003). Traditional lamps were

phased out due to their mercury content and low energy efficiency based on directives in Europe (Cogeneris sprl, 2011). Some parts of these directives are related to the environment. As the public becomes more conscious of the environment, corresponding legislations might be released in the future. The processes or materials that result in pollutions would face restrictions from legislation or the society. Environmental friendly level of materials could represent the possibility that the materials would become inaccessible in the future. The second part concerns the situation in which materials cannot be accessed. It is also the part that most examined studies mentioned. This part is divided into two blocks in this thesis: suppliers and surroundings. In terms of suppliers, following aspects were considered: diversity of suppliers, location of each supplier, relationship between the company and its suppliers, price offered by each supplier, and inner problems of each supplier. In terms of surroundings, following eight branches were considered. Competition from other sectors, especially the defense sector, might limit the access to certain materials during national security emergencies or war. Dependence on other markets can also restrict accessibility. For example, when the main product of mining is reduced or stopped, its by-product will also be reduced or stopped. Global reserve show the amount of a material which can be economically explored. When the reserve of this material is large, the potential available amount of this material is high too. Geo-relationship between supplying countries and the country where the company is located can also influence the accessibility of materials sometimes. The 2-month interruption in exports of REEs from China to Japan in 2010 is a good example of georelationship's influence (Ramzy, 2013), as is the case of oil shock from Arabic countries to countries supporting Israel in 1973 and 1979. At the same time, the stability of supplying countries can influence materials' accessibility. For example, when copper-cobalt mining areas were invaded in Zaire in the 1970s, its supply of cobalt was suspended (Alonso, 2010). Although there were other reasons for disruption of the cobalt supply, the stability of supplying country affected accessibility of materials. Besides stability, demands inside the supplying countries, priority to satisfy local companies, strikes and corresponding legislative reforms can also influence accessibility of materials. The ratio between global demand and supply (sum of global production and stocks) can affect the supply accessibility at global level. When the global demand of one material is much higher than its supply, it is likely more difficult for an individual company to obtain that material. At the end, the recycling rate can represent the potential supply amount of materials available from urban mines.

#### 2.3 Imbalance between demand and supply

The demand and supply in this dimension is the amount directly related to the actor – the company who produces the product. Demand amount here means the needed amount of each material to satisfy the target production amount of the product. The supply amount here means the amount that the specific company can have access directly at that moment, including the actual supply amount and the potential supply amount from its actual suppliers and potential suppliers. Any material with a greater supply than its demand is significantly less worrisome than a material with a small demand but less supply. Hence, it is the imbalance between demand and supply which needs to be considered for criticality rather than demand or supply individually.

## 2.4 Dynamic aspect or abrupt changes

The fact that situations change suddenly is more disturbing than the situations themselves. Situation here means the whole set of things that are happening or the conditions that exist at that particular time, which includes the price, reserve amount, reserve location, geo-relation between involves countries and every other thing which is related to the criticality of that material. Solutions would be found within enough time and the market responds to material criticality issues, only time matters. For example, after the cobalt crisis, Zambia and Australia significantly increased their cobalt production. Zaire decreased its highest market share of cobalt from 70% in 1978 to 31% in 2004. Cobalt substitutes were developed for applications such as magnets, cutting tools, ceramics and paints (Alonso, 2010). Hence, time that the market needs to receive a new balance and time that the company needs to adapt to the new situation is vital since some companies might not survive a material crisis. In addition, criticality can be indeed projected differently at different times and in different situations. The trigger of the rare earth crisis of 2010 was different from that of the palladium crisis of 1990s. The solution regarding to the fact of "projected differently" is to find a list that contains impact parameters of criticality of all possibilities (Figure 8) - impact parameters pool. One material crisis can be caused by impact parameters A, B, and C while another material crisis can be caused by impact parameters D, E, and F. The idea is that all impact parameters A, B, C, D, E, F and others are in the same pool so that we are aware to get prepared. Thus, we can select the most severe or possible impact parameters to assess criticality based on the specific situation while maintaining a close eye on the others. Hence, the first approach to interpret dynamic factors is through a scenario where appropriate impact parameters from the above pool are chosen according to that specific situation. An originality of this approach is that it is the first time that criticality evaluation methodology offers different choices of impact parameters or indicators during evaluation.

The dynamic aspect has already been considered by several studies (Knoeri, Wäger, Stamp, Althaus, & Weil, 2013; Komal, 2015). Our second approach to interpret the dynamic factors is through indicators. It is difficult to separate dynamic perspectives from indicators since some indicators are dynamic themselves in nature and evolve over time (Komal, 2015). Certain impact parameters also represent a potential risk such as environmental regulations resulting in a ban or opposition by clients.

The third approach to interpret dynamic factors is through weighting or threshold settlement in the evaluation model. For example, we can chose to calculate the criticality by assuming 20% or 30% of the candidates are considered critical. We can also follow the expertise to set the threshold. One place in the evaluation model is left for users to adjust the thresholds or weightings themselves according to their own situations while some suggestions and guidelines for setting those values have been offered.

## **1.1 Conclusion**

At the end, here is the definition proposed for the criticality of materials in this thesis: *The criticality of a material is a relative value due to the interaction among the importance of the material to the object, the imbalance between demand and supply, and accessibility of the material. Criticality is reinforced with abrupt changes or situations where actors are not able to adapt.* In detail, all materials are important somehow. The word "relative" means that the importance of other materials is not neglected but only the most important ones, which can cause huge damage to the actor, make the actor not able to adapt to the new situation or need urgent attentions, are highlighted. The word "object" projects the dynamic concept of criticality by stating the particular situations, i.e. to which the criticality of materials is analyzed: a product and which product, a group of materials and which group, a technology and which technology, a company and which company, a country and which country etc. It also shows the scope of the study. The word "actor" projects the organizations behind those objects. For example, if the object means a product, then the actor can be the company who produces this specific product or other corresponding participants which are involved in reactions to adapt to the new situations.



Figure 8 : Impact parameters from the diagnosis part

## **CHAPTER 4**

# **CASE STUDY OF RARE EARTH CRISIS**

This chapter aims at giving a deep look about materials crisis happened in the history and giving a supplementary instruction for the previous chapter. The objectives of this case study are: 1) to better understand criticality mechanism; 2) to seek inspirations for defining or determining the criticality; 3) to know how materials issues influence society; 4) to confirm the conclusions of the diagnosis chapter.

## 1. Introduction of rare earth materials

Rare earth materials are the ores, oxides, metals, alloys, semi-finished products or components containing rare earth elements (REE). REEs include 17 metal elements from the IIIB group of the period table: Scandium (Sc), Yttrium (Y), Lanthanum(La), Cerium (Ce), Praseodymium (Pr), Neodymium (Nd), Promethium (Pm), Samarium (Sm), Europium (Eu), Gadolinium (Gd), Terbium (Tb), Dysprosium (Dy), Holmium (Ho), Erbium (Er), Thulium (Tm), Ytterbium (Yb) and Lutetium (Lu). Among them, the last fifteens are lanthanides whose atomic number is from 57 to 71. The atomic number is 21 for Sc and 39 for Y. Scandium's chemical properties are quite different to others and it makes its usages different to others. Besides, Pm is radioactive and we can find barely in Nature, neither in the rare earth ores. Those elements are also divided into light rare earth elements (La, Ce, Pr, Nd, Pm, Sm and Eu) and heavy rare earth elements (Gd, Tb, Dy, Ho, Er, Tm, Yb, and Lu) (刘光华, 2007).

In fact, rare earth elements (REE) are not rare neither on Earth. The name came from a misunderstanding of the era when the REEs were found. In 1789, a Swedish amateur mineralogist C.A. Arrhenius found a rock in the village "Ytterby" near Stockholm. Hence, he named the rock "Ytterby ore". In 1794, a finish chemist J. Gadolin analyzed this ore and he couldn't recognize 2 fifth of the elements inside. He did experiments and found that the solid oxides of these elements with metallic luster are insoluble in water. He also named the ore "Yttria" and the element contained inside "Yttrium". At that moment, the solid oxide which is insoluble in water used to be called "earth". And they thought the "Yttria" ore is rare. That is how the "rare earth" comes from. However, there are more than one metal in the "Yttria" ore.

In 1842, a Swedish chemist C. Mosander discovered two other elements in this rock: Erbium and Terbium. Until 153 years after the rock has been found, all 17 rare earth elements were discovered.

Due to the special optical, electrical, and magnetic properties that most of other elements do not possess, rare earth elements are widely used in the high technologies. They are also called industrial vitamins. In the list of 35 high-technical elements announced by the U.S. Department of Defense, 16 were rare earth elements (only Pm was not included). In the 26 high-technical elements announced by the Japan Science and Technology Agency, 16 were rare earth elements. From previous parts, we know that rare earth materials were often designated critical by European or American organizations. That is the reason why I decided to do a case study on rare earth materials.

#### 2. Materials' properties

As stated previously, the importance of material is partly related to the functionality that materials offer. The function is then related to the properties of materials. Hence, we can learn what makes rare earth materials so demanded by current high technologies from this section.

# 2.1 Atomic structural characteristics of rare earth elements

Among the lanthanides, the radius of atom is decreasing from Lanthanum (0.1879nm) to Lutetium (0.1734nm) in general. The radius of element Y is 0.1801 nm, which is around the middle. The radius of Sc (0.1641nm) is smaller than all lanthanides' but still very close to them. Sc and Y have similar outer electron structure. Although Sc and Y don't have 4f electronics, their out electron structure is the one of  $(n - 1)d^{1}ns^{2}$ . That makes their chemical properties similar as the lanthanides'. It is also the reason why Sc and Y are divided into rare earth elements. The tiny difference of electron levels and ionic radius of those rare earth elements is one of the reasons which make their properties similar. That's also one of the reasons why they are difficult to be separated.

In terms of chemical reactions, REEs tend to lose three electrons (one of 5d, one of 6s and one of 4f) and become positive trivalent ions. Under certain conditions, they can also be in +2 or +4 charge state. Their valence variation is the theory base for redox separation method. For example, we can oxidize preferentially the Ce in order to separate it with other rare earth elements. REEs with +2 or +4 charge state have special properties compared to their normal

+3 charge state. They can be used to produce semi-conductor, magnetic materials or luminescent materials. Most REEs have a hexagonal closepacked structure, including Sc, Y, Gd, Tb, Dy, Ho, Er, Tm, and Lu. La, Pr, Nd and Pm have double hexagonal closepacked structure. Ce and Yb have face-centred cubic structure. Sm has its unique diamond structure.

# 2.2 Physical properties

Rare earth elements have typical metal properties. Except that Pr and Nd show lightly pale yellow, all elements are silver shiny metal (see Figure 9). Their densities are from 2.992 g/cm<sup>3</sup> (Sc) to 9.842 g/cm<sup>3</sup> (Lu) while the majority of them are between 6 to 8 g/cm<sup>3</sup>. Many of them have very close physical properties, such as melting point, boiling point, heat capacity (constant pressure), electronegativity etc. Coupled with the fact that rare earth ores contain usually more than one element, it is difficult to separate them.



Figure 9 : Lanthanum metal
Image source: http://images-of-elements.com/lanthanum.php

# 2.3 Electrical properties

Rare earth metal has low conductivity. At room temperature (25°C), all rare earth metals have high resistivity with a value between 50 ~ 135 (x10<sup>-4</sup>  $\Omega$ \*cm) except for Yb. It is 1 to 2 magnitudes higher than copper or aluminum's resistivity.  $\alpha$ -Lanthanum becomes superconducting at 4.6K.  $\beta$ -Lanthanum becomes superconducting at 5.85 K. The radiuses of REE ions are larger than other ions, so they are less attractive to anions. The majority of rare earth compounds have ionic bond. These compounds are well conductive.

## 2.4 Optical properties

The 4f electron layer of REE is shield by outer  $5S^25P^6$  electron layer. Except for La 3+ (4f<sup>0</sup>) and Lu 3+ (4f<sup>14</sup>), 4f electrons of other REEs can be arranged arbitrarily in seven 4f orbitals. It generates various spectral phases and levels. When 4f electrons jump from different energy levels, they can absorb or emit radiations at various wavelengths. The absorption, emission and fluorescence spectrums provide the basis for research or application of REE luminescent materials.

## 2.5 Magnetic properties

Magnetic comes from the movement of electrons inside the materials. The magnetic of REE is closely related to the 4f electrons' movement and to their crystal structures. At room temperature, the majority of rare earth metals are paramagnetic. With the decrease of temperature, they are becoming ferromagnetic or antiferromagnetic. Some rare earth compounds have high saturation magnetization. Some rare earth compounds have high anisotropy constant. Some rare earth compounds have high magnetic telescopic. In rare earth researches, it is discovered that superconductivity of some rare earth compounds does not coexist with diamagnetic, but coexist with ferromagnetic (ErRh<sub>4</sub>B<sub>4</sub>, HoMo<sub>6</sub>S<sub>8</sub>) or antiferromagnetic (RERh<sub>4</sub>B<sub>4</sub>, RE = Nd, Sm, Tm; REMo<sub>6</sub>S<sub>8</sub>, RE = Gd, Tb, Dy, Er). Although rare earth compounds have above excellent magnetic properties, their Curie temperature is much lower compared to other metals like Fe, Co etc.

## 2.6 Chemical properties

Due to their large atomic radius and the ability to easily lose the electrons of 4f, 6s and 5d, rare earth elements are strongly chemically active just after the alkali metals. The order of reactivity among REEs is showed as the figure below:



Figure 10 : chemical activity trend of rare earth elements

As they are very active, pure rare earth metals need to be contained into kerosene, especially for light rare earth elements, or into wax. That is why we find rare earth oxide ore in Nature instead of pure metal. That also makes the recycling and refinement more difficult.

## 3. Supply chain of rare earth materials

### 3.1 World reserve and production distribution

According to the USGS on-line data, rare earth mines or deposits were found all around the world, except for Antarctica and Arctic (see Figure 11). According to Google Earth, rare earths are even found in the Moon. According to the figure below, deposits are slightly more concentrated along the coastlines of continents such as south east of Asia, east of South America, east west of the Africa, North America and Australia. More deposits may exist and not have been discovered yet. In addition, there are resources existing in the ocean. With development of technology and improvement of economic profitability, they may be exploited one day in the future as well. In addition, the relative abundance of rare earths elements in the Earth's upper continental crust is higher than Hg, Ag, In etc. Some of REEs are higher than W, Sn etc. To conclude, rare earths are not rare and the current impression that they are only concentrated in China is false.



Figure 11 : Rare earth element mines, deposits, and occurrences. Details are available on USGS on-line spatial data ('Rare earth element deposits: interactive map', 2014)

Among the reserves discovered until now (see Figure 12), China, U.S. and Commonwealth of Independent States (CIS) or former Soviet Union were three countries which hold the most reserves from 1995 to 2012.



Figure 12 : Worldwide reserve of rare earth oxide from 1995 to 2013 (based on the data from USGS) (USGS, 1994to2014)

Start from 2012, the data of CIS is integrated into "others" group in the figure. Large amount of reserves were discovered in Brazil since 2012 which made China, Brazil and "Others"

contain the most rare earth reserves in the world now. However, reserves amount in the U.S. remains almost the same compared to 1995. Due to the discoveries of new rare earth mines or deposits, some countries occurred lately in the Figure 12.



Figure 13 : Worldwide rare earth oxide mine production from 1995 to 2013 (based on the data from USGS) (USGS, 1994to2014)

The figure above shows the worldwide rare earth oxide mine production amount from 1995 to 2013. Before 1995, the U.S. was the country dominating rare earth production in the world. Then the production center moved to China due to mine cost, high local labor cost compared to China, high pollutions caused by mining activity and opposition from local people. In 1995, the U.S. still produced almost as many as China. But three years later, China has been dominating the production till now. Meanwhile, India has been producing around 2700 tons every year except of a huge raise from 2005 to 2007.

After combing reserve and production data, Figure 14 was generated to show their relation. From 1995 until 2013, the annual world rare earth oxide (REO) production is always more than 66 000 tons. However that production amount is negligible compared to reserve amount. Reserves amount was 1600 times of production in 1998. Even in the worst time -2006, reserve amount was around 600 times more than the production. The peak' appeared in Figure 14 may be one of the causes of peak\* in Figure 13. India was reacting to the global market. When there was few production compared to reserve, it increased the production amount in order to satisfy the market demand. In 2013, REO reserve was around 1200 times of its production. From Figure 12 and 13, we can also see that both REO world reserve and production are both slightly increasing in a general trend. To sum up, we can suggest that the world REO reserve can satisfy our demand for a long time if there is no emerging demand. The depletion of REO resources is not an urgent issue at this moment. One challenge here may be exploiting these reserves technical feasibly and economic profitably without causing too much environment burden.



Figure 14 : Comparison of Worldwide REO production and reserve from 1995 - 2013

Based on above data, contribution of countries which possess reserves regarding rare earth oxide production can be extracted (see Figure 15). From the figure, we can see that Malaysia's contribution rate is relatively high within consideration of its reserve proportion in the world. According to this figure, Malaysia, China and India are basically contributing more in the REO world production compared to its reserve ratio. In another word, these countries are producing much higher than other countries based on the ratio of reserves they have. On one hand, if they continue this high contribution rate, their reserves have higher acceleration speed to meet depletion. On another hand, it may not be feasible to require all the countries contributing equally because the return of asset for exploiting small deposits is much lower than big ones, not mentioning the requirements of whole supply chain and market behind. Due to lack of information, data of some countries are missing for several years, so they are represented as blank in the figure. Evaluation method of contribute rate is stated below.



Figure 15 : Rare earth oxide production contribution of different countries based on its reserve ratio (data based on the calculation of data from USGS)

The vertical axe if the contribution rate (CR) is:

Eq.(1)

$$CR = \log(\frac{(production \ of \ country \ i)/(world \ total \ production)}{(reserve \ of \ country \ i)/(world \ total \ reserve)})$$

For example, when one country produces 50% of REO while it is holding 50% of reserve too, the CR is equal to 0. When one country' production ratio is smaller than its reserve ratio, its CR is a negative number. When prod ratio/ resv ratio is smaller (while its CR is negative), its CR has higher absolute value. When one country' production ratio is larger than its reserve ratio, its CR is a positive number. When prod / resv ratio is larger (while its CR is positive), its CR has higher absolute value too.

#### 3.2 Rare earth export and import situation

In this section, two countries' rare earth import and export situations were explained: China and the United States (U.S.). The reason to select China is because it is dominating currently the production and it is one important key to 2010 rare earth crisis. The U.S. was selected due to its high demand of rare earths and being the country of the highest Gross Domestic Product (GDP) in the world. According to Figure 16, China is exporting much more rare earth products than importing. Combing with section IV of this chapter (history of China rare earth industry), we can tell that the majority of its import are primary rare earth materials while the majority of its import are high technology involved rare earth products.



#### Figure 16 : China rare earth products export and import history from 1996 to 2009 (data source: (PEI & Kong, 2011))

According to figure below, the U.S. is importing more than exporting, but its trade deficit is smaller than China's. According to the USGS report, their imported products include cerium compounds, ferro-cerium / alloys, mixed rare-earth chlorides, mixed REOs, REOs compounds, rare earth metal / alloys and thorium ore (monazite or various thorium materials). Their exported products include cerium compounds, rare-earth metals / alloys, other rare-earth compounds, ferro-cerium / alloys, and thorium ore (monazite or various thorium materials). Among them, four products are both in the import and export list. One of the reasons may be that these products in the export list have higher grade or quality. The U.S. imported the raw materials or low grade materials from China, process then export them. Another reason may be these products contain different elements and answer to different demands. For example,

the bastnäsite ores of Mountain Pass in California are Ce and La concentrated while lateritic ores of southern China are Y and La concentrated.



Figure 17 : U.S. rare earth products export and import history from 1996 to 2013 (data source: USGS)

## 3.3 Uses of rare earth materials

Rare earth materials are used in many different areas, such as high-technique equipment, agriculture, defense, bio-medical etc. According to the USGS ('REE - Rare Earth Elements - Metals, Minerals, Mining, Uses', n.d.,), 65% of rare earth materials are used for chemical catalysts; 19% are used for metallurgy or alloys; 9% are used for permanent magnets; 6% are used for glass polishing and 1% for other in the Unites States in 2013. Combined with their properties, table below showed main applications.

Table 7: Properties of rare earth element and their corresponding functionality and application based on « 稀土材	料学»
(刘光华, 2007)	

Properties	Functionality	Application case
4f electrons' spin arrangement	Hard magnetic	Permanent magnets
4f electrons' spin arrangement	Magneto-optical feature	Bubble memory, optical isolator, magneto-optical recording device
4f electrons' spin arrangement	Huge spin	Magnetic Resonance Imagining (MRI) contrast material
4f electrons' spin arrangement	Entropy control	Magneto-frozen
4f electrons' spin arrangement	Huge magneto-impedance	Magnetic sensors
4f electrons' spin arrangement	Superconductivity and magnetic coexistence	High critical magnetic field of superconductors
4f orbitals electronic transitions	4f-4f activate phosphor	Red or green phosphor, fiber amplifier, in vitro diagnostic reagents
4f orbitals electronic transitions	4f-5d activate phosphor	Blue phosphor, electroluminescent substance
4f orbitals electronic transitions	4f-4f solar light receiving luminescent centre	To improve the efficiency of the Silicon solar battery
No distortion of substrate' crystal structure after the introduction of activator	Substrate	Magnetic bubble memory material of substrate of lasers and luminescent material
Improve the sintering feature and dielectric feature	Electroclash and dielectric	Light adjustment material and transparent material
Glassy form Structural properties and hydrogen-pro	Low-loss optical fiber Hydrogen storage	Optical fiber Hydrogen storage alloy

## 3.4 End life of rare earth products

Rare earth materials are often used in high technological devices which are often difficult to be dismantled. These applications often need very small amount of rare earth and their high chemical activity has been mentioned previously. Above reasons make it difficult to recycle rare earth materials. For now, rare earth recycling technology or market is still not mature. Only 1% of rare earth is recycled in general (Graedel et al., 2011). However, more economic profit of rare earth and high imbalance between demand and supply may encourage the recycling sector of these materials.

# 4. History of rare earth industry in China (extracted from «中国稀土保卫战 » (王珺之, 2011))

# 4.1 Chronic of China rare earth activity

Activities which are non-Chinese but important for understanding the global rare earth industry are marked in gray.

1949: A huge amount of rare earth deposits were discovered at Mountain Pass in the U.S.

1950s: Large amounts of rare earth were discovered in Bayan Obo mine by Zuolin He. It was estimated as 80% of the world rare earth reserve at that moment.

1950s: Rare earth extraction was integrated into national science plan by President Enlai Zhou.

1962: Beijing General Research Institute for Nonferrous Metals established an experimental plant. They were using ion exchange and half countercurrent extraction process to produce the single rare earth oxides at laboratorial level. Until 1962, 16 single rare earth oxides preparation methods were developed. They were served as basis for future rare earth metallurgical plant.

1960s beginning: Changsha 602 plant, Shanghai Yuelong chemical plant and Baogang 8861 plant were built. It meant that China Rare earth industry passed to industrial level from laboratorial level. However, the rare earth production process and technologies in China were far behind the one of the U.S. Hence, the majority export of rare earth materials of China were rare earth mines. At the same time, China was importing high-technique involved rare earth products from other countries. The high level rare earth production methodologies were industrial confidentiality at that moment.

1972: Guangxian Xu and other researchers received a mission from the government to get high purity of Pr and Nd from separation process. They improved the extraction separation process by combining proper extraction and complexing agents to generate quaternary ammonium salt – diethylenetriaminepentaacetic acid (DTPA) push-pull system. Xu is also regarded as the father of rare earth industry in China.

1974: The industrial scale trial to extract the rare earth based on the push-pull system theory developed by Guangxian Xu succeeded.

1975: Guoping Huang of Guangzhou nonferrous metal research institute developed a method of ore concentrates by using hydroxamic acid. Six years later, Baogang plant applied this method and made the production capacity of high purity rare earth exceeded 10 000 tons.

1976: Guangxian Xu proposed the cascade extraction theory. It was then applied across the country. The extraction process of rare earth in China then became advanced in the world. The application of push-pull system and cascade extraction theory made Chinese rare earth industry much more competitive than before.

1978: The 3<sup>rd</sup> Plenary Session of the 11<sup>th</sup> Central Committee of the Communist Party of China highlighted the rare earth industry development in China. And a National Rare Earth Promotion and Application Office was built. After then, the government paid more attention to rare earth industry than before. A China Society of Rare Earth was established next year. All those measures promoted the development of rare earth industry in China.

1985: Ganzhou Nonferrous Metal Institute and Jiangxi University completed a new method (ammonium sulfate – ammonium carbonate precipitation process) which decreased significantly the cost of extraction of rare earth. It was widely used in the extraction of ion adsorption type rare earth ore at industrial level.

1965-1985: The U.S. dominated all stages of rare earth material processing.

1990s: Due to the reform and opening policies in China, some medium and small state-owned enterprises were transformed to private enterprises or joint venture. More and more private enterprises were built as well.

1998-2005: The decline period of the U.S. rare earth industry.

2007-now: The U.S. rare earth industry restarted.

On one hand, support from the government, mastering of know-how, reform and opening policies, profit-push and large rare earth reserves stimulate the development of the rare earth industry in China. On the other hand, cost increase, environmental constraints and national resource strategy made rare earth industry in the U.S. shut down or moved to China. The production center transferred from the U.S. to China. This transfer started from 1980s and completed around 1990s. Until now, China has still been the production center of rare earth industry. However, the U.S. and some other countries have restarted existed old mines or opened new mining sites of rare earth materials. At the same time, Chinese government put export quota in the rare earth industry. The environment (such as increase of labor cost and environmental constraints) to produce rare earth materials in China is no longer as good as before. Although China is the leader in rare earth oxide production and its techniques to extract rare earth are among the best, its techniques of rare earth deep processing and fine chemicals are not as good as its extraction's.

## 4.2 Related policies of the largest supplier - China

From the history of China rare earth industry, we can see that Chinese government has been playing an important role in this sector.

1950s-1990s: The government was strongly supporting the rare earth industry.

1991: Rare earth minerals were designated as one of the protective mineral species by Chinese government.

1999: China started the export quota for rare earth materials.

2004: The export tax rebate of rare earth metals was decreased from 13% to 0.

2004: The export tax rebate of organic compounds of rare earth mixture was decreased from 15% to 5%. The export tax rebate of inorganic compounds of rare earth mixture was decreased from 17% to 5%.

2006: The total production amount of rare earths was controlled by the Chinese government.

2007: Chinese government started charging a 10% of export tax for rare earth products.

2007: New foreign-owned mines are forbidden in China, but the cooperation between foreign and Chinese companies was allowed. The investment or cooperation for rare earth deep processing, new rare earth materials and applications were encouraged.

2010: The total rare earth export quota decreased 30% in China.

1996-2011: The environmental regulations for rare earth industry were: "Integrated wastewater discharge standard" (GB8978-1996), "Integrated emission standard of air pollutants" (GB16297-1996) and "Emission standard of air pollutants for industrial kiln and furnace" (GB9078-1996).

2011- : The environmental regulations for rare earth industry has been "Emission standards of pollutants from rare earth industry" (GB26451-2011). This regulation is stricter than three previous ones.

# 4.3 Possible motivations of protective policies regarding rare earth in China

The main official arguments of export restrictions stated by China in the WTO dispute were to protect the environment and to avoid resource depletion in China. Mining activities do damage significantly the ecosystem and have huge impact to human health. Mining emissions contain lots of chemicals, especially radiation contamination pollution of certain radioactive elements emitted by rare earth mining. With the development of society, people have higher and higher requirements concerning the environment. If we draw lessons from the U.S. rare earth industries, environmental concerns will probably be one reason which will decrease the economic feasibility or even impede the mining activity, production or relating activities. Based on current data, China did lose its reserve weight of rare earths from 85% in 1992 to 36% in 2009.

Except for official arguments above, China has other motivations to bring stricter policies on rare earth mining. Firstly, illegal mining has been bothering the Chinese rare earth industry for a while. The illegal mining activities usually contain larger security risk. In terms of efficiency rate, stat-owned mines' is 60%; private mines' is 40% and illegal mines' is just 5% (王珺之, 2011). They are making huge waste of rare earth ore resources. At the same time, illegal activities increase the opacity of information which is not good for resources management. Secondly, there are two other sources for consumers to get the supply: smuggling and quota reselling still allow rare earth being sold to other countries. If the legislation and law enforcement become stricter, these two supply sources may be eliminated. Thirdly, China's rare earth industries are located in the upper stream of the rare earth industrial activities. The downstream sections were dominated by other developed countries like the U.S., the EU, Japan, etc. China's rare earth industries lack of innovation and have hysteresis of high-technologies. That explained why China encouraged foreign countries investing in cooperation of downstream rare earth materials or innovation. Fourthly, the rare earths' prices were under estimated to China. Points above showed the problems remained in the Chinese rare earth industries and they also showed motivations for potential reform in the mining area.

### 5. Recent international attentions to rare earths

#### 5.1 Diaoyu (in Chinese) / Senkaku (in Japanese) Island dispute

The sovereign dispute over Diaoyu / Senkaku Island between China and Japan was a historical issue dated from the 20<sup>th</sup> century. Then a boat collision incident in 2010 led to a high tension between these countries. In the same year, China suspended the rare earth export to Japan for several months. After China cutting its export quota of rare earth materials, some countries or industries suffered from lacking of rare earth materials which could not ensure the production of certain products. Despite the deny of Chinese government, one Japanese manager from rare earth related trading company stated that China cut the rare earth export to punish the Japanese government regarding its reaction to the island dispute (Ramzy, 2013).

#### 5.2 WTO rare earth dispute

In March 2012, the U.S. conducted a request for consultations concerning China's restrictions on export of rare earths, tungsten and molybdenum which were against the agreements of the WTO. Later, 18 other countries joint the dispute as the third parties. The main arguments of China for the restriction were to reduce the pollutants and to protect its exhaustible resources. The other side disagreed and argued that it was for downstream Chinese industries having protected access of those materials. They were also disagreed with the relation between restrictions and environment in this case. For now, the U.S. won the dispute.

# 5.3 Rare earths were designated as critical materials by the U.S., the E.U. and some other organizations

Hatch (2011), Rademaker et al.(2013) and Massari & Ruberti (2013) regarded rare earth materials as critical by default and then focused on those materials' supply and demand situations or strategies. The U.S. (Department of Energy, 2010)(Department of Energy, 2011)(National Research Council, 2008)(OUSDATL, 2013) and the EU (European Commission, 2010) (European Commission, 2014) have designated rare earths as critical materials more than one time.

More details are stated in chapter 2.

## 5.4 Price roller-coaster of rare earths

Price is one important indicator which partly shows how market reacts to one material. There is a roller-coaster in the price of rare earth materials from 2007 to now (see Figure 18). The majority of materials returned to their original prices such as Tb, La and Ce or have at least dropped comparing to their peak values such as Nd and Pr. We can see that the price of rare earths increased significantly in general started from 2004 to 2011 (see Rhodium's price history - part c of Figure 18), its price increased around 22 times from December 2003 to June 2008. Then it decreased 90% from June 2008 to January 2009 in a short time. The other two figures showed the same phenomenon for 10 rare earth oxides with a peak around 2011. The swift growth of rare earth appeared in 2010 may be the market's response to China's rare earth exportation policy. This important price change was also a trigger of those critical materials studies.



Figure 18 : Rare earth oxides' price history in US dollar from 2007 to 2014 – Part "a" with high price. Part "b" with lower price (Haque et al., 2014). Part "c": Market price of Rhodium from Jan 2000 to Jan 2014 (source: Kitco website)

#### 6. Reflections of criticality regarding causes of rare earths crisis

The unique properties of rare earth elements made them difficult to be replaced. The technologies progress made rare earth materials being used in various important areas, especially in defense and high-tech industries. What's more, those products which contained rare earth elements are still needed and will be needed by the society for a while. In the future, some other elements might become technically, economically and socially feasible to replace the rare earth elements. However, most of them remain irreplaceable at this moment regarding the performance they offered. From previous paragraphs, we can see that there are enough reserves compared to the current production requirement for a long time without significant change. If we consider resource amount in Earth's crust, they are not rare at all. Despite that rare earths are often by-product of other minerals' production and rare earth mining is a heavy polluting activity, the supplying countries can still produce them if other conditions allowed. Hence, the reserve amount or resource depletion is not the predisposition of recent rare earth issues or tense atmosphere related to rare earths. China's export disruption is the trigger which made us consider rare earths critical; however, it is still not the whole reason. From the Figure 12 we can see that China's rare earths reserves is less than half of the world. Other countries have large amount of reserves and certain possess also technologies (like the U.S. and France who have produced rare earths before) to produce rare earth oxides. From Figure 15, we can see some countries' contribution rates of rare earth oxides production are very low. They are potential suppliers or the countries that can produce more in the future. With more and more strict environmental regulations and labor cost, the total cost of rare earth production might become higher in the future. The plants might transfer to other countries which was the case that the U.S. rare earth industries declined and moved to China in 2000s.

The causes of recent rare earth issues are as below: 1) Importance of rare earths materials to certain industries or countries. It can be showed by excellent performance offered by the unique properties of rare earths. At the same time, their main use areas like defense or high-techniques are sensitive to a country. They may relate to strategic level of a country. 2) The imbalance between demand and supply. This cause reflects two levels. Firstly, it reflects the need of products contained rare earth by current society. Defense, high-technique and other sectors need rare earths. And countries or people need products of those sectors. Secondly, it reflects the imbalance between demand and supply of rare earth materials. For example, while China cut its rare earths export to Japan around 2010; Japanese companies did not have enough supply from its Chinese or other suppliers. One thing to be highlighted is that a
consumer usually keep at least two or three suppliers. It is a strategy that most companies applied. China was not the only supplier; however the supply amount from other countries plus the amount from smuggling and quota selling could not satisfy the demand of Japanese consumers. At the same time, the industries in China could get supply amount as usual. It was hence the imbalance between the demand amount and accessible supply amount of corresponding actor (Japanese industry that needs rare earth materials). 3) The accessibility to supply. The reason why Japan could not get the rare earths from China at that moment was because that Chinese government cut the export to Japan. It was not due to the supply amount inside China. In another word, it was due to the accessibility to supply. Except for the motivations of protective policies listed above, another possibility is that China used rare earths as a political tool on island dispute with Japan. 4) Sudden changes and potential risks. Even though China started protective policies long time ago and China is still holding its protective policies for rare earths, it was the only moment in the history that export to Japan was completely cut. The reaction that China cut all export quota of rare earth to Japan can be considered as a sudden change. Due to the occasional tense political relation between Japan and China, the supply suspend from China to Japan could have been considered as a potential risk before it really happened. Possible scenarios should be made. On another hand, a concentration of supplying source was also a cause. In 2010, around 90% of Japan's rare earths supply came from China. The concentration of supplying source increased the supply risk. To sum up, despite the scope of reflection is at regional level (China, Japan etc.), it matches the metabolism of criticality of materials to a product which was stated in the previous chapter.

## **CHAPTER 5**

## DEVELOPMENT OF "Materials Criticality Profiling Methodology (MCPM)" AT PRODUCT LEVEL

I have heard some researchers saying that all materials are important and it makes it useless to focus on criticality. To answer this point of view, I agree that all the materials are important somehow and no material will be critical forever because market will solve the problem itself. However, even if no material would be permanently critical in the future, some materials have already been critical in real situations. Even if criticality is a relative notion and all materials are important, we still need to find those critical ones due to the limit of time, financial or human resources. The study of criticality can make resource division more optimal in the following ways: stockpiling, R&D orientation etc. Critical material studies can be regarded as a reflection of the market to solve corresponding problems. To be carried out in advance, their results can be used to prevent industries or countries from suffering critical materials issues.

Based on diagnosis of criticality, this chapter described a methodology called "Materials Criticality Profiling Methodology (MCMP)" that can be used to alert and evaluate the critical materials at product level by industries as a decision-making support tool. Product focus is a unique point of this methodology. Further, this methodology allows personalization in different situations by projecting dynamic factors into indicators and scenarios. One basic scenario is given as an example to demonstrate how to build criteria for calculation from information supported by the diagnosis part.

## 1. Introduction

As stated in the introduction chapter, studies on critical materials and resources are very important to global industry and economy. Based on the review, it lacks a product-level evaluation methodology. Currently, there are evaluation methodologies for criticality developed for specific regions (Department of Energy, 2010; European Commission, 2010), for specific groups of metals (Nassar et al., 2011), for technologies with a specific perspective (Komal, 2015) and for material markets (Poulizac, 2013). For industry, the results from above evaluations and studies cannot be used directly if the goal is to determine which materials are critical for their own products. For example, beryllium was designated as a critical resource

by the EU (2010), however, this information is not useful for companies that do not require beryllium in their products or that are not located in the EU. The list of critical materials was designated from a list of candidates in a European study. Hence, different pools of candidates will result in different lists of critical materials. In addition, the focus of critical material studies at product level is different from those for specific regions or a specific group of materials, not mentioning the involved different geographical information.

## 2. Materials and methods for developing the methodology

## 2.1 Overview of evaluation methodology

This criticality evaluation methodology is designed for production industries at product level. The guidelines of how to implement this methodology are shown in Figure 19 below.



Figure 19 : Guidelines of how to implement criticality assessment methodology

The first step is to decide the target product for analysis, such as a battery, permanent magnet, lighting emitting diode, etc. The second step is to decide the material candidate pool. As one product might consist of thousands of materials, analysis might take too much time or resources. Thus, this step allows selection of materials of interest without exceeding capacity (e.g., budget or human resources). We can also analyze all materials related to the product if possible. The third step is to build the scenario. We can have following scenarios as example: Basic, Forecast, Potential risk, Environment, Legislative, Economic, and Innovation etc.

These scenarios are related to the strategies of the company. For example, if the company's finance situation is not good, it might build the Economic scenario where the impact parameters related to economy are highlighted and have bigger weights. On the contrary, if the company has a very good finance state and it wants to have a better environmental or innovative image, it can then build a scenario of Environment or Innovation. Each type has its own priority / preference, which consists of a list of selected impact parameters (IPs) (which might lead to different criteria) or weightings of criteria (see following paragraph). The scenarios allow for multi-decision making and grants criticality of materials under corresponding priority. Scenario building reflects the scope of assessment. The fourth step is the selection of indicators for certain impact parameters, as there are many indicators available to evaluate some impact parameters. The objective of this step is to allow users to adapt their studies to specific situations, and this step makes possible to improve the methodology over time with accurate potential indicators. When data on an indicator is not available, users can choose another one. This also allows the comparison of different results under different indicators. For example, eco-toxicity and climate change give completely different results in assessing the environmental friendliness of a material. After these four steps, the model, including the calculation box, provides a list of inputs. The fifth step involves entering the data as well as weightings required by the calculation model, after which the model will offer three outputs: a general score of criticality for each material, a diagram showing the details for all materials (what contributes more to criticality), and mitigation measures for corresponding issues. The mitigation measures can be extracted from existing studies and then added by experts in the corresponding domains.

The criticality in the final diagram is represented by "criteria", which is different than impact parameters. A criterion can represent criticality by assembling proper impact parameters. A criterion might contain more than one impact parameter, and one impact parameter might involve more than one criterion. The impact parameter and criterion are differentiated to make the model be able to adapt to different situations. For example, the IP "supplying ratio of one supplier" influences both the criterion "quality of relationship with suppliers" and the one of "geo-relationship". However, this IP is not appropriate to assess criticality as an individual criterion. When the input of supplying ratio changes, the calculation formula of the above two criteria does not need to be changed. Instead, one can simply change the input data. Figure 20 below shows how the impact parameters are connected to the criteria in the basic scenario.



Figure 20 : Connections between impact parameters and criteria in the basic scenario

## 2.2 Calculation of criteria of basic scenario

This section shows a basic scenario covering most influential impact parameters and possible to be evaluated nowadays. Readers may view the basic scenario as an example for the development of others by adding or removing indicators.

Firstly, the model's calculation contains five variables for creating scenarios: Materials in the candidate pool, Suppliers of materials, Substitutes, General functionality, and Functionality. General functionality and functionality are differentiated since more than one hierarchy is needed to understand the functionalities of complex products. Extraction of variables is carried out for automation of the model. The dependency of a specific company on its required materials in each specific situation can be determined. Below are mathematical symbols for those variables, which are used for calculation of criteria as well as for the framework of the model.

 $M_i$ , i = 1 to N; Materials in the candidate pool to be analyzed. There are N materials in total.

 $S_i$ , i = 1 to X; Suppliers of materials. There are X suppliers in total.

 $Stt_k$ ,  $_k = 1$  to Y; Substitutes. There are maximum Y substitutes of materials.

 $GF_L$ ,  $_L = 1$  to Z; General functionality offered by materials for the product. There are Z general functionalities in total.

 $F_l$ ,  $_l = 1$  to H; Functionality offered by materials to the product. There are H functionalities in total.

In detail, *N*, *X*, *Y*, *Z* and *H* are the numbers of each variable. For example, if there are two materials to be analyzed, then N = 2 with the two materials represented by  $M_1$  and  $M_2$ .

Secondly, some inputs are in the form of text to give information:

CL : Company location

P: Product name

M<sub>i</sub> : The i<sup>th</sup> Material's name

 $R_{(M_i)}$ : The i<sup>th</sup> Material's mass ratio in the product

S<sub>j</sub>: The j<sup>th</sup> supplier's name

L<sub>(S<sub>i</sub>)</sub>: The j<sup>th</sup> supplier's location (city and country)

 $F_{(M_i)}$ : The functionality offered by the i<sup>th</sup> Material

F<sub>l</sub>: The l<sup>th</sup> functionality

GF<sub>L</sub>: The L<sup>th</sup> general functionality

Thh.  $U_{(F_1)}$ : The threshold's unit of l<sup>th</sup> function

## Criterion 1: Imbalance between demand and supply

This criterion is calculated based on the ratio between the amounts of supply and demand for a material. The following symbols are used to represent their meanings in the calculations.

 $SR_{(S_j-M_i)}$ : Supplying ratio of  $S_j$  for  $M_i$  $D_{(M_i)}$ : Demand amount of  $M_i$  $S_{(M_i)}$ : Supplying amount of  $M_i$ AoP: Target producing or purchasing amount of product P  $R_{(M_i)}$ : The i<sup>th</sup> Material's mass ratio in the product LoP: Production loss of product P  $ASA_{(M_i-S_i)}$ : Available supplying amount of  $M_i$  from  $S_j$ 

As shown in Eq. (2), the demand amount for the  $i^{th}$  materials can be calculated from the planned production amount of the product as well as the percentage of the contained material by rectification with production loss.

Eq.(2)  
$$D_{(M_i)} = AoP \times (1 + LoP) \times R_{(M_i)}$$

The supply amount of each material can be summed from the available supplying amount that the company's suppliers can offer (see Eq. (3)).

$$Eq.(3)$$
$$ASA_{(M_i)} = \sum_{1}^{X} ASA_{(M_i - S_j)}$$

The imbalance between demand and supply of  $M_i$  can be calculated as below in Eq. (4).

$$\frac{D_{(M_i)}}{S_{(M_i)}} = \frac{AoP \times (1 + LoP) \times R_{(M_i)}}{\sum_{j=1}^{j=X} ASA_{(M_i - S_j)}}$$

On the other hand, if the company already has data on demand or supply, they can directly use their ratio rather than applying equation 4.

## Criterion 2: Value (functional and economic) of this material to the target product

This criterion is a combination of functional value and economic value. In terms of functional value, we need to 1) establish a functionality table for each material offered to the product (like Table 8) and 2) conduct a survey of experts for weighting.

Table 8 : Functionality contribution of each material to the product

GF1	<u>General Functionality 1 ( l= 1 to )</u>
F1	The 1st functionality
F2	The 2nd functionality
F <i>l</i>	The <i>l</i> th functionality
GFL	<u>General Functionality L (l = to)</u>
F( <i>l</i> +1)	The ( <i>l</i> +1)th functionality
n	The n <sup>th</sup> functionality

A functionality profile for each material to be analyzed for the product should be established at first. After determining general functionalities (e.g., physical properties, thermal properties, magnetic properties, etc.), we can determine all functionalities offered by each material (e.g., hardness, density, physical carrier, etc. for physical properties).

Then we can conduct a survey using technical experts, designers, or clients in order to determine functionality, including GF and F, for each material. The Analytic Hierarchy Process or Delphi's method can be used for weighting.

In the survey, experts provide the percentage that each material contributes to functionality. The functional value of the i<sup>th</sup> material to the product is shown as follows:

Eq.(5)

$$FV_{(M_i)} = \sum_{1}^{H} Con_{(M_i - F_l)} \times W_{(F_l)}$$

With:

 $FV_{(M_i)}$ : Functional value of the i<sup>th</sup> material to the product  $Con_{(M_i-F_l)}$ : Contribution of M<sub>i</sub> to the functionality F<sub>l</sub> in the product W<sub>(Fi)</sub>: Weighting (Importance) of the functionality F<sub>l</sub> to GF<sub>L</sub> in the product

In terms of economic value, the cost to purchase this material for producing the total product is used.

Economic influence of the  $i^{th}$  material is as shown in Eq. (6):

$$EI_{(M_i)} = \sum_{j=1}^{X} \left[ SA_{(M_i - S_j)} \times Price_{(M_i - S_j)} \right]$$

With:

 $EI_{(M_i)}$ : Economic influence of the i<sup>th</sup> material  $SA_{(M_i-S_j)}$ : Supplying amount (purchasing amount) of  $M_i$  from  $S_j$ Price<sub>(M\_i-S\_j)</sub>: Price of M<sub>i</sub> offered by S<sub>j</sub>

In the end, the "Value" is represented by the association between functional value and economic influence (without money unit), as shown in the following formula:

Eq.(7)

Eq.(6)

$$V_{(M_i)} = FV_{(M_i)} \times (EI_{(M_i)}/\$)$$

#### Criterion 3: Substitutability of the material to the product

Poulizac (2013) used cost and performance (related to the properties of a material) to represent the substitute, which covered functional and economic aspects. One material might satisfy these two requirements but still at laboratory level. If the material cannot be industrialized within a very short time or the company lacks the proper equipment or labor force to adapt to new process, then it cannot replace the actual material. Thus, more time or

research is needed for production technology to come mature, and the technological maturity of substitutes should be considered. After becoming technically and economically feasible to manufacture, the substitute may become supply restricted as well. This will lead to another similar criticality assessment. To simplify the assessment, I recommend only analyzing resource depletion of the substitute instead of carrying a second criticality evaluation. At the end, whether or not a substitute candidate is eligible is evaluated by comparing the reference (actual material being used / the material to be analyzed) and its substitute candidates in terms of functionality, technology maturity, price, and resource depletion.

Functionalities were specified and weighted in previous criterion (Table 8). They can be used to analyze both the reference material and its substitutes. The threshold of functionality can be a setting according to the technique specifications. The judgments from technique experts provide the minimum requirements for functionality. If the substitute candidate's properties satisfy the entire threshold, then it can be considered as an eligible substitute. Technological maturity can be obtained by surveys from corresponding experts. Delphi's method is a good tool to determine technological maturity. Price can be used to represent the economic aspect when the whole cost for applying the substitute is unknown. The resource depletion ratio (RDR) can be imported from the Eco-invent database. At the end, the two following points are examined to determine the substitutes; 2) combined with substitutability satisfaction of each eligible substitute. This represents the degree that the substitute matches the minimum requirements to become eligible.

Next, the calculation of the i<sup>th</sup> material's substitutability was presented as an example. Firstly, the functionally eligible substitutes should be designate. We need firstly check the functionalities contributed by the reference material. Then, we need to check whether or not the substitute candidate's measurement values of these functionalities satisfy thresholds, i.e., the measurement value should be higher than the minimum threshold of performance required or lower than the maximum threshold of performance required. If a substitute candidate is not functionally eligible, no further calculation is needed.

The second step is to calculate the substitutability satisfaction of above designated ones. In terms of functionality, we need firstly to calculate the functionality satisfaction with weighting (FSW) of the substitute candidate by comparing experimental measurements values of the substitutes and the threshold.

Eq.(8)

$$FSW_{(F_l - Stt_k)} = \left| \frac{MV_{(F_l - Stt_k)} - Thh_{F_l}}{Thh_{F_l}} \right| \times W_{F_l}$$

With

 $FSW_{(F_l-Stt_k)}$ : Functionality satisfaction with weighting of functionality  $F_l$  of materials  $Stt_k$  $MV_{(F_l-Stt_k)}$ : Measurement value (MV) of  $F_l$  of substitute  $Stt_k$  $Thh_{F_l}$ : Threshold settled for the functionality  $F_l$ 

Then we can use exponential functional to treat  $FSW_{(F_1-Stt_k)}$  to obtain the General Functionality's FSW.

$$FSW_{(GF_L-Stt_1)} = \overline{\sum_{lmin(L)}^{lmax(L)} e^{FSW_{(F_l-Stt_1)}} \times W_{GF_L}}$$

The reason to use exponential function is to eliminate the negative value and still reflect the relative relationship between negative values and positive values.



Figure 21 : Exponential function diagram

On one hand, when the value of "functionality satisfaction with weighting of one detailed function" (corresponding to "x" in the figure above) is negative, it means: 1) it fails to attend the threshold and 2) how much it failed to attend the threshold. Above all, those with negative values here have less satisfaction than those with positive values. On the other hand, the "functionality satisfaction with weighting of one general function" is the integrated value of all its sub-functions. Hence, the EXP() value makes it possible to better present their relations. We calculate the total functionality satisfaction of the eligible substitute  $FSW_{(Stt_k)}$  by averaging all related functionalities.

Eq.(10)

Eq.(11)

$$FSW_{(Stt_k)} = \sum_{l=1}^{H} FSW_{(F_l - Stt_k)}$$

Similarly, we obtained the general functionality satisfaction  $FSW_{M_i}$  of the reference material.

$$FSW_{(M_i)} = \sum_{l=1}^{H} FSW_{(F_l - M_i)}$$

Then, we should compare  $FSW_{(Stt_k)}$  to  $FSW_{(M_i)}$  in order to obtain the relative functionality satisfaction (RFS) of the substitute.

Eq.(12)

$$RFS_{Stt_k} = \frac{FSW_{Stt_k}}{FSW_{M_i}}$$

Technological maturity can be marked by experts as a percentage. A value of 100% means that the technology is totally mature. Then, we need to compare the technology maturity (TM) of the substitute to that of the reference material.

In terms of economics, we first benchmark the cost for using the substitutes  $C_{Stt_k}$  and reference material  $C_{M_i}$ .

Eq.(13) 
$$C_{Stt_k} = M2R_{Stt_k} \times PoM_{Stt_k}$$

With

 $C_{Stt_k}$ : Cost of substitute with equivalent of 1 kg of reference material  $M_i$  $M2R_{Stt_k}$ : Mass of k<sup>th</sup> substitute needed compared to 1 kg of reference material  $PoM_{Stt_k}$ : Price of material  $Stt_k$  per kg.

After determining the cost of substitute, it is to calculate the cost difference  $CD_{Stt_k}$  between using the substitute and reference material. When  $CD_{Stt_k}$  is positive, a higher absolute value means that the substitute has better economics. When  $CD_{Stt_k}$  is negative, a lower absolute value means better economics.

Eq.(14)

$$CD_{Stt_k} = \frac{C_{M_i} - C_{Stt_k}}{C_{M_i}}$$

With

 $CD_{Stt_k}$ : Cost difference between substitute  $Stt_k$  and reference material  $M_i$ 

Then, we use the exponential function to solve the negative or positive problem while calculating the economic accessibility (EA) of the substitute according to the following formula.

Eq.(15)

$$EA_{Stt_k} = e^{CD_{Stt_k}}$$

In terms of resource depletion, we can calculate the relative RDR of the substitute to its reference material. Similar to economic accessibility, a positive  $RDRBR_{Stt_k}$  means a higher absolute value and improved contribution to substitutability. When  $RDRBR_{Stt_k}$  is negative, its lower absolute value means improved contribution to substitutability.

Eq.(16)

$$RDRBR_{Stt_k} = \frac{RDR_{M_i} - RDR_{Stt_k}}{RDR_{M_i}}$$

With

RDRBR: Resource depletion ratio benchmarking with the reference material

Then, we use the exponential function to solve the negative or positive problem according to the following formula.

Eq.(17)  
$$Exp(RDRBR_{Stt_k}) = e^{\frac{RDR_{M_i} - RDR_{Stt_k}}{RDR_{M_i}}}$$

Exp(RDRBR): RDRBR's exponential function value

By combining above four terms, we can obtain the general evaluation of the performance of the substitute material  $Stt_k(GESP_{Stt_k})$  as follows:

Eq.(18)

$$GESP_{Stt_k} = \overline{\left(RDB_{Stt_k} + EA_{Stt_k} + TM_{Stt_k} + RFS_{Stt_k}\right)}$$

With

 $RDB_{Stt_k}$ : Resource Depletion Benchmarking. It is equal to  $Exp(RDRBR_{Stt_k})/Exp(RDRBR_{M_i})$  $TM_{Stt_k}$ : Technology Maturity of substitute k

Therefore, the substitutability of  $M_i$  after considering all substitutes can be integrated as equation (19).

Eq.(19)  
Substitutability = 
$$\sum_{k=1}^{Y} (GESP_{Stt_k})$$

#### **Criterion 4: Environmental friendly level**

A low environmental friendly level means the material damages more the environment according to selected indicator, for instance human toxicity, eco-toxicity or global warming potential (GWP). At the same time, the public are more and more sensitive to the environment. This makes industries pay more attention to environmental damages caused by their products. Materials that cause higher environmental damage (lower environmental friendly level) would face more problems due to social pressure, environmental restrictions, eco taxes etc. in the future. This criterion aims to show the possibility of having these problems. Human toxicity, eco-toxicity, and GWP are suggested as three possible indicators for this criterion. The company can chose one or their average as the indicator to show the contribution of this criterion to the criticality. The values of these three indicators can be obtained from a database such as Eco-invent.

#### Criterion 5: Legislation ban or hinder level

For this criterion, we need to establish a legislative inventory for each material based on the standards showed in the table below by collecting legislative information in the product sector. This criterion is inspired by the mercury limitation in the lighting system based on the EU RoHS Directive (2011/65/EU). A similar case can occur in other materials for other products. The material might become critical if it is forbidden to be used. The solution is similar to other critical materials: looking for substitutes, decreasing or eliminating demand for this

material or even changing the product design; however, we do not need to increase the supply amount, find better suppliers or find stable supplying countries. Based on the above standards, we can become aware of the legislative risk, which can stimulate similar problems of criticality.

Table 9 : Legislation ban or hinder level marking standards

Source: In	ventory of legislation in the sector of the product
Note	Description
1	There is a legislative (laws, directive etc.) ban or the usage of this material is hindered in the corresponding sector in the geographic area related to the product for a short time.
0.75	There is a legislative (laws, directive etc.) ban or the usage of this material is hindered in the corresponding sector in the geographic area related to the product activities for a medium-long time.
0.50	There is a high possibility that the material will be banned or hindered by legislation in the corresponding sector in the geographic area related to the product activities for a known time.
0.25	There is a low possibility that the material will be banned or hindered by legislation in the corresponding sector in the geographic area related to the product activities for a known time.
0	There is no legislative (laws, directive etc.) ban or the usage of this material is not hindered in the corresponding sector in the geographic area related to the product activities for a known time.

# Criterion 6: Quality of relationship with suppliers including diversity of suppliers (concentration of suppliers)

The important role played by suppliers is sometimes underestimated by companies. Suppliers can influence companies in the following aspects: quality, timeliness, competitiveness, innovation and finances (Reiss, 2010). After considering these aspects, the following key points were extracted to evaluate the quality of the relationship with suppliers.

- a. Quality of supplying product  $(QoM_{S_j})$ : quality of supplied materials from supplier  $S_j$  directly affects quality of products the company will produce.
- b. Timeliness  $(TIM_{S_i})$ : delivery time of  $S_j$ .
- c. Innovation  $(Inn_{S_j})$ : effort that suppliers  $S_j$  make for innovation. Companies can take advantage of innovative materials offered by suppliers by becoming more competitive.
- d. Exchange  $(Xch_{S_j})$ : an exchange between the company and its supplier  $S_j$  in terms of company strategies, newsletters, and perspectives.

e. Human  $(HF_{S_j})$ : humans are a vital factor in purchasing or business dealings. A reliable and royal partner (human) assures the quality of the relationship between two companies.

Source:	Interview wit	h department of	purchase		
Note	Quality of supplying materials	Timeliness	Innovation	Exchange	Human
0	Excellent quality	Always in time	Strong innovations strategy, innovated end product (materials)	Deep and comprehensive exchange	Reliable, royal, responsible
1	Bad quality	Always late	No innovations at all, no plan to stimulate innovation neither	No exchange at all	Shady, personal conflicts

Table 10 : Standards for marking the relationship with suppliers

This table shows the standards for giving scores to the six factors mentioned previously. Firstly, we should establish a relationship profile of each supplier by requiring the purchase department to make above standards. Secondly, we combined the quality of relationship with supplier  $(QRS_{S_j})$  with its supplying share for material  $(SR_{(S_j-M_i)})$ . Finally, this criterion - quality of relationship with suppliers of  $M_i$  material  $(QRS_{M_i})$  is obtained by averaging all suppliers' relationships for each material.

Eq.(20)

$$QRS_{S_j} = \overline{\left(QoM_{S_j} + TIM_{S_j} + Inn_{S_j} + Xch_{S_j} + HF_{S_j}\right)}$$

$$QRS_{M_i} = \sum_{j=1}^{X} SR_{(S_j - M_i)}^2 \times QRS_{S_j}$$

#### **Criterion 7: Depletion of reserves**

This value can be obtained from database like Eco-invent. We can also calculate the value based on the ratio of production and reserve amount of each mineral or raw material. If the material is synthetic, we can use the ratio between production amount and capacity.

Eq.(22)

#### Depletion of reserve = DoR

 $= \frac{Global \ production \ amount \ of \ material \ (or \ related \ minerals)}{Global \ reserve \ amount \ of \ material \ (or \ related \ minerals)} = \frac{GProd_{M_i}}{GRsv_{M_i}}$ 

## Criterion 8: Geo-relation (political and bilateral economic exchange) between supplying and buying countries

This geo-relation involves how two countries (countries of supplier and buyer) get along with each other both politically and economically. More economic exchange reduces risk of conflicts between two countries. If there is some territorial dispute or historical conflict, the policies of the two countries may influence the commercial relationship between companies. Sometimes, import or export is ongoing even during tense bilateral political relations, which is why bilateral economic exchange must also be considered. To determine the geo-political relationship between two countries, geopolitical or international diplomatic experts must be interviewed based on below standards (Table 11). We can also apply Delphi's method to approach a consensus. For economic bilateral exchanges, following factors were considered: a) export, b) import, c) tourist revenue, d) stock investment of the buying country in supplying countries, e) stock investment of supplying countries. The money amount can be obtained from government documents, e.g., France diplomatic official site (French Gov., 2015a) for France-related bilateral economic exchange.

Table 11 : Standards for geo-political relation scores inspired by China diplomatic ranking system.

Source:	Interview with	n geopolitical	or internationa	l diplomati	ic experts and	designers
		• •		•	•	

Note	Description
1	War
0.75	Relation
0.5	Partnership
0.2	Traditional good partnership
0	Ally / Union

Since higher diplomatic scores contribute more to bad bilateral political relations and higher money exchanges contribute more to good bilateral economic relations, we can use Eq. (23) for the geo-relation calculation.

Eq.(23)

$$Geo-relation = \frac{Diplomatic \ score}{Economic \ bilateral \ exchange \ (M \ \$)}$$

#### Criterion 9: Global demand to supply ratio

This criterion is calculated based on the ratio of global demand to supply. The global supply amount is the sum of global production and stock amount of a material.

Eq.(24)

Global demand and supply ratio = 
$$\frac{\text{Global Demand Amount}_{M_i}}{\text{Global Supply Amount}_{M_i}}$$

Alonso et al. (2012) developed an evaluation methodology for the demand and supply ratio of REE and reported methods and different scenarios to forecast demand and supply. Their method can also be used in this criticality evaluation methodology.

#### Criterion 10: Stability of supplying country

For stability of the supplying country, four possible indicators were collected: ease of doing business (World Bank, 2016), fragile states index (FFP, 2015), estimated political stability by country (Quandl, 2015) and worldwide governance indicator (World Bank, 2014). The scores of "ease of doing business" rank the conditions of doing business in 189 countries. This index includes following factors: starting a business, dealing with construction permits, registering property, getting credit, protecting investors, paying taxes, trading across borders, enforcing contracts, and resolving insolvency. The index is released by the World Bank every year. The smaller score represents better business conditions. The indicator "fragile states index" shows the fragility ranking of 178 countries and was created by the Fund of Peace. The results are released every year. "Estimated political stability by country" is an indicator of the political stability of 188 countries / regions. It was obtained from the database "Quandl". A higher value indicates a more politically stable country. Finally, "worldwide governance indicator' shows the quality of governance of more than 200 countries whose results are released every

year. It has also been used by the EU in their critical materials study (European Commission, 2010). This indicator considers a) voice and accountability, b) political stability and absence of violence, c) government effectiveness, d) regulatory quality, e) rule of law, and f) control of corruption. The score ranges from 0 (worst governance) to 100 (best governance). As their scales are different, the order of the value of each indicator should reflect the same physical meaning in order to make them comparable (i.e. when the value decreases, the conditions become better. They are enlarged or shorten into the same scale: 0 -100).

#### **Criterion 11: Recycling rate**

The recycling rate here represents the percentage of materials that can be recycled. It is frequently stated as a measure to mitigate the criticality issue (Poulizac, 2013) as a higher recycling rate and more urban mines lead to a more available supply. This indicator has also been considered by some criticality evaluation studies (European Commission, 2010) (Öko-Institut e.V., 2009). It can be obtained from existing studies, e.g., the USGS (2016) mineral reports, United Nations environment program's recycling rates report (Buchert, Manhart, Bleher, & Pingel, 2012) and other academic studies (Graedel et al., 2011).

## 3. Results

## 3.1 Presentation form for evaluation results

The 11 criteria listed above have different physical meanings and units. We need three steps to make them comparable. Firstly, we need to put them into the same order. This means that when the value of each criterion increases, it contributes more to criticality. Secondly, we take the relative value of each criterion. It is obtained by Eq. (25).

Eq.(25)

Relative value of each criterion = (value of criterion - threshold)/threshold

After the previous data were treated, there are positive and negative values from the calculation above. Hence, the third step makes them all positive or remained within certain range. Here, two options were proposed. The first option uses an arc tangle function, which can make all values remain into the range of  $\pi$  (from  $-\frac{2}{\pi}$  to  $\frac{2}{\pi}$ ) and the threshold of all criterion become the same value. We can adjust the interval to make all values positive, for

example, transfer the values to a range between 0 and  $\pi$ . The second option is the exponential function, which makes all values positive and is easier to be presented in a radar chart as shown previously (Poulizac, 2013). All thresholds become "1". Finally, we adjust the results with weightings of criteria.

Besides the radar chart, we can obtain a general score for each material. The general score means the relative value of criticality of each material compared to others. The results are only valuable under specific conditions of each study by specifying the following information of the product: its suppliers, supplying share, functionality offered by this material for the product and so on.

For the third output, recommendations for the mitigation approaches, we need to establish a database on mitigation measures which have been recommended by existing studies at first. Then, we need to connect them to each criterion and impact parameters. We can then look only the corresponding mitigation measures of criteria which have surpassed the threshold.

## 3.2 Completeness and sensitivity

The evaluation methodology contains numerous impact parameters. However, not all can be covered in each study due to lack of data, human resources, budget and other constraints. The coverage of the impact parameter under each dimension can be used to show the uncertainty of the study.

Taking the coverage of the dimension "imbalance between and supply" as an example. According to the diagnosis (Figure 8), this dimension was divided into "demand" and "supply in which "demand" has three impact parameters and "supply" has two impact parameters. If only one impact parameter is covered under "demand" in a case study, then its coverage is 33%. Similarly, if one impact parameter is covered under "supply", then its coverage is 50%. Thus, we can obtain the coverage of "imbalance between and supply" by combing "supply" and "demand" as: $33\% \times 0.5 + 50\% \times 0.5 = 42\%$ . Same for two other principal parameters: importance and accessibility to supply.

In terms of sensitivity, the same proportion change of the same input of all materials will not influence the relative criticality of materials when the change doesn't surpass the interval of inputs and the inputs are non-zero. Hence, analyzing the sensitivity by changing one input of one material individually is recommended.

## **CHAPTER 6**

## VALIDATION

## Part I A THEORETICAL APPLICATION ON PERMANENT MAGNET

## 1. Introduction

This chapter is about the first case study which has been conducted to demonstrate the MCPM and test its feasibility. It also served to improve the calculation model and complete the details which were not considered during methodology conception.

The target product is permanent magnet which is an object produces its own persistent magnetic field. In another word, a permanent magnet can spontaneously afford a suitable flux in the air gap of a device. It is achieved by processing magnetized materials which have suitable characteristics. Permanent magnet is used in following devices: direct current, stepper, synchronous motors, moving coil, holding force actuators, sensors etc., which is widely used in modern industry and very important to many technologies (Campbell, 1996). The application requires a lot of confidential data which companies were not willing to share. Without cooperation of a company, it is impossible to conduct an application for the MCPM proposed in this thesis. Hence, a scenario is based on a hypothetical company. A part of data was referenced from similar situations. When data were not available, they are derived from similar sources in order to complete the demonstration.

Structure of this chapter is as below: 1) Basic information and scenario introduction. 2) Data collections which were divided into material, technical, supplier and geographical related profiles. 3) Calculation of each criterion. 4) Intergradation of above criteria's and final results presentation. 5) Completeness analysis of this application.

## 2. Scenario and data collection

## 2.1 Scope and scenario

The hypothetical company "Magnet Expert Co." is a professional permanent magnet manufacturing company which is located in France. Their star-product is called "Super magnet" whose annual production amount is 100 ton. It is the RE-Fe-B type permanent material. The main raw materials for producing the magnet is rare earth materials (Nd) 36%,

iron 63%, boron 1% and so on (刘光华, 2007). With around 10% of materials loss during the production, they purchase usually 40 tons of rare earth materials and 70 tons of irons for producing 100 tons of "Super magnets" every year. Their customer base is the electronic industries, including the microwave devices, aerospace dedicated and electronic instrument.

As the first application, I picked up neodymium and iron as candidates due to following reasons: 1) two materials are enough to show how the model works; 2) fewer materials to be analyzed equals to less time and data; 3) the two candidates comprise 99% of the mass of target product – "Super magnet"; 4) two candidates are different and contrastive with the fact that neodymium is a rare earth element which has been designated critical in some recent studies and iron is a massive produced material which is used very broadly. Hence, two materials has been analyzed in this study, where N = 2. Their detailed names are as follow with each one being given a code  $M_i$ , *i* is from 1 to 12.

Hence,  $M_1$  = Neodymium (rare earth element),  $M_2$  = iron.

The scenario selected is the basic one which is stated in the methodology chapter. After scenario type having been chosen, the impact parameters (see Figure 20) and calculation model are determined as well.

## 2.2 Data collection

#### Materials profile to produce one LED

The annual production amount of permanent magnet is assumed 100 tons in the hypothetical company "Magnet Expert Co.". With the mass proportion of each material and production loss ratio stated previously, the demand amount of each material is as below:

Demand amount (planned to purchase) of neodymium:

 $100 \times (1 + 10\%) \times 0.36 = 40$ 

Demand amount (planned to purchase) of iron:

 $100 \times (1 + 10\%) \times 0.63 = 70$ 

Table 12 : Materials profile of permanent magnet

Code	Unit	<i>i</i> = 1	<i>i</i> = 2
	/	<i>M</i> <sub>1</sub>	<i>M</i> <sub>2</sub>
M <sub>i</sub>	/	Neodymium	Iron
$R_{(M_i)}$	%	36%	63%
<b>D</b> <sub>(M<sub>i</sub>)</sub>	tons	40	70
GRsv <sub>Mi</sub>	tons	140 million	169 300 million
$GProd_{M_i}$	tons	0.11 million	3 091 million
Human toxicity	kg 1,4-DCB-Eq /1kg of material	709.96	577040000
Recycling (end of life recycling rate)	/	1%	72%

Global reserve and production amount of neodymium (rare earth (USGS, 1994to2014) and iron (USGS, 2015a) in the table above are from the USGS annual report. The end of life recycling rate of iron is 52%, 67%, 78% or 90% according to different studies (Graedel et al., 2011). The average is

$$\frac{(52\% + 67\% + 78\% + 90\%)}{4} = 71.75\%$$

The end of life recycling rate of neodymium is less than 1% (Graedel et al., 2011).

There are three indicators proposed for environmental friendly level:

Indicator 1- Human toxicity;

Indicator 2 - Eco-toxicity;

Indicator 3- GWP 100a

Table 13: Environmental impacts of iron and neodymium (based on Eco-invent 2010)

	Unit	Method	Iron	Neodymium					
Human	kg 1,4-DCB-	ReCiPe Midpoint (E)/human toxicity:	577040000	709.96					
Toxicity	Eq	1							
Eco toxicity	kg 2,4-D-Eq	TRACI/environmental impact: 6 US	16588000	11.73					
GWP 100a	kg CO2-Eq	EDIP2003 w/o LT/global warming	14396000	38.487					
		w/o LT: 3 GLO							
Iron: no	<i>Iron:</i> no. 22 - metal/extraction – mine – iron - GLO – unit - infra. Yes								

Neodymium: no. 1 - chemical/inorganics - neodymium oxide, at plant - CN - kg - infra. No

The reason why neodymium has much fewer impacts than iron is because it is a by-product of other metals, so the impacts of neodymium were shared with its main-products' production. And its main product took the majority share of the impacts.

I assumed that the company chose the human toxicity as an indicator to calculate the environmental friendly level of its materials. Environmental impacts of iron and neodymium according to these indicators are showed above.

## **Technical profile of Permanent magnet**

This technical profile was analyzed under three general aspects: physical, thermal and magnetic properties of permanent magnet. For each aspect (general functionality), several main properties were extracted as functionalities in this application.



Figure 22 : Functionalities structure diagram of permanent magnet

After the functionalities structure being determined, their weightings were given with below standards.

 Table 14: Standards of functionality weighting in permanent magnet application

Source: Interview with technical experts and designers or client					
Note	Description				
1	The function offered by this material to this product is very important				
0.5	The function offered by this material to this product is meaningful, but replaceable				
0	The function offered by this material to this product is negligible				

Magnet is an alloy of iron and rare earth, so the functionality of each material is an integrated result of whole alloy's property. In this case, the importance of functions offered by iron and rare earth are considered both very important.

Table 15: Weighting results of functionalities of permanent magnet (Note: the values below were determined by author for the sake of calculation facility which means the results can not represent weightings of permanent magnet's functionalities in other case)

Functi	onality contribution of each material to the product	Weight	Fe	Nd
GF1	Physical Properties / Functionality ( i = 1 to 3)	<u>0,01</u>	0.97	0.03
F1	Physical carrier	1	1	0
F2	Hardness	0,1	1	0
F3	Density	0,6	0.9	0.1
GF2	<u>Thermal Properties / Functionality (i = 4)</u>	<u>0,8</u>	0.3	0.7
F4	Maximum service temperature	0,8	0.3	0.7
GF3	Magnetic Properties / Functionality (i = 5 to 9)	<u>1</u>	0.34	0.66
F5	Curie temperature	1	0.3	0.7
F6	Maximum energy product (BH) max	1	0.4	0.6
F7	Residual Induction Br	1	0.2	0.8
F8	Residual magnetic flux density	0,8	0.4	0.6
F9	Coercivity	1	0.4	0.6

In the table above, the right two colons show the contribution of each material to each function of the product. For example, iron contributes 1 (100%) to the F1 (Physical carrier) while neodymium contributes 0. In terms of the F7 (residual induction Br), iron contributes 0.2 (20%) while neodymium contributes just 0.8 (80%). The note  $_{(1)}$  means that the value is

the average of its sub functions. For example, iron contributes 0.97 (97%) of the general function - physical properties / functionality where the value 0.97 is the average of F1, F2 and F3. 0.97 = (1+1+0.9)/3

So the function value offered by iron is:

 $0.01 \times 0.97 + 0.8 \times 0.3 + 1 \times 0.34 = 0.59$ 

The function value offered by neodymium is:

 $0.01 \times 0.03 + 0.8 \times 0.7 + 1 \times 0.66 = 1.22$ 

Based on the properties of materials, praseodymium, samarium and mixed rare earth were selected as candidates to substitute neodymium in permanent magnet so as cobalt, manganese, chromium and nickel as candidates to substitute iron. The data of critical materials candidates and substitute candidates were listed in the two tables below (Table 16 and 17).

When i = 1,  $M_1$  is neodymium, and its substitute candidates are:  $Stt_1 = praseodymium$ ,  $Stt_2 = samarium$ , and  $Stt_3 = mixed rare earth$ .

When i = 2,  $M_2$  is iron, and its substitute candidates are:  $Stt_1 = cobalt$ ,  $Stt_2 = manganese$ ,

and  $Stt_3 = chromium$ , and  $Stt_4 = nickel$ .

Table 16: Substitutability data of Neodymium in Permanent magnet (Note: figures in orange were imaged based on the reference materials' information for the sake of calculation facility). Data of Nd2Fe14B's functionalities (cells F4:F12) were from a book about rare earth materials wrote by 刘光华(2007). Maximum service temperature of NdFe14B (F7 cell) is from a magnet website (e-Magnets UK, n.d.). Data of Pr2Fe14B were from 刘光华(2007) and Eclipse Magnet(n.d.). Dataof cells G6 and G8 were also from 刘光华(2007). Data of cell G7 was from Poggiani (2009). Data of cell G9, G10, G12 was from Zhang et al. (2012). Data of cell G11 was from Benabderrahmane (2013). Line 13 the price of materials was the corresponding metal on line price in 21 December 2014. Line 14 mass needed compared to reference was based on the atomic mass of corresponding elements. Line 15 resource depletion data were from Eco-invent databases.

А	В	С	D	E	F	G	Н
1			Reference	- Actual product	S	ubstitute candidates	;
2	2 Neodymium (Nd)			Neodymium (Nd)	Praseodymium (Pr)	Samarium (Sm)	Mixed Rare Earth (MRE)
3		Threshold	Threshold unit	Nd2Fe14B	Pr2Fe14B	Sm2Fe14B	MRE-Fe-B
4 F1	Physical carrier	S	Solid	S	S	S	S
5 F2	Hardness	80	Hv	100	250	200	500
6 F3	Desity	7	g/cm3	7,4	7,47	7,5	7,2
7 F4	Maximum service temperature	100	°C	150	358	300	200
8 F5	Curie temperature	450	°C	583	564	570	250
9 F6	Maximum energy product (BH) max	70	kJ/m3	289	73,9	300	150
10 F7	Residual Induction Br	1,15	Т	1,31	1,18	1,1	1,18
11 F8	Residual magnetic flux density	1,15	Bt/T	1,23	1,35	1,38	1,19
12 F9	Coecitivity	200	KA/m (HcB)	880	211,4	900	150
13 Price of r	naterials (metal, not oxide) (21 dec 2014)		\$ /kg	87,00	175,00	20,00	29,80
14 Mass nee	eded compared to reference - 1kg of Nd		kg	1,00	0,98	1,04	0,97
15 Resource	e depletion ratio of material (ecoinvent)			3,50	3,60	5,20	2,00
A	В	С	D	E	F	G	Н

Table 17: Substitutability data of Iron in Permanent magnet. (Note: figures in orange were imaged based on the reference materials' information for the sake of calculation facility). Data of Nd2Fe14B's functionalities (cells F4:F12) were from a book about rare earth materials wrote by 刘光华(2007). Maximum service temperature of NdFe14B (F7 cell) is from a magnet website (e-Magnets UK, n.d.). Line 13 the price of materials was the corresponding metal on line price in 21 December 2014. Line 14 mass needed compared to reference was based on the atomic mass of corresponding elements. Line 15 resource depletion data were from Eco-invent databases.

	A B	С	D	E	F	G	Н	I	
1	1		Reference	- Actual product		Substitute candida	ates		1
2	Iron (Fe)			Iron (Fe)	Cobalt(Co)	Manganese (Mg)	Chromium (Cr)	Nickel (Ni)	2
3		Threshold	Threshold unit	Nd2Fe14B	Nd2Co14B	Nd2Mn14B	Nd2Cr14B	Nd2Ni14B	3
4 F1	Physical carrier	S	Solid	S	S	S	S	S	4
5 F2	Hardness	80	Hv	100	90	120	400	500	5
6 F3	Desity	7	g/cm3	7,4	8,5	7	6,7	7,4	6
7 F4	Maximum service temperature	100	°C	150	200	100	170	140	7
8 F5	Curie temperature	450	°C	583	560	480	500	490	8
9 F6	Maximum energy product (BH) max	70	kJ/m3	289	200	185	60	100	9
10 F7	Residual Induction Br	1,15	Т	1,31	1,21	1,2	1,11	1,15	10
11 F8	Residual magnetic flux density	1,15	Bt/T	1,23	1,2	1,01	1,1	1,02	11
12 F9	Coecitivity	200	KA/m (HcB)	880	800	180	200	300	12
13 Price	of materials (metal, not oxide) (21 dec 2014)		\$ /kg	0,89	32,50	2,35	7,80	16,13	13
14 Mass	needed compared to reference - 1kg of Nd		kg	1,00	1,06	0,98	0,93	1,05	14
15 Reso	urce depletion ratio of material (ecoinvent)			1,00	1,01	76,60	24,90	12,50	15
	A B	С	D	E	F	G	Н		

#### Supply profile

Six suppliers were created for this application. Their information like price and location is inspired from real market. Companies' names and their available supplying amounts are fabricated.

In terms of rare earths (Nd), the suppliers are "Jiatong" (supplier 1), "Rare-earths" (supplier 2) and "Jinshu Materials" (Supplier 3).

 $S_1$ : Jiatong Co. is located in Jiangxi, China. The purity of rare earth oxides materials is 99.99%. The rare earth they are supplying is  $\pm 350/kg$ .

 $S_2$ : Rare-earths Co. is located in Texas, USA. The rare earths materials they are supplying is USD 60/kg.

 $S_3$ : Jinshu Co. is located in Shanghai, China. The rare earths materials they are supplying is  $\pm 330/kg$ .

In terms of iron, the suppliers are "Ruide Iron" (supplier 4), and "Jinshu" (Supplier 3).

 $S_4$ : "Ruide Iron" is located in Jiangsu, China. The iron they are supplying is  $\pm 620$ /kg.

 $S_3$ : Jinshu Co. is located in Shanghai, China. The iron they are supplying is  $\frac{Y}{600}$ /kg.

There are also two more possible suppliers for iron. Details are available in the table below. The total numbers of suppliers is 6 in this study which means X = 6. The suppliers,  $S_j$ , j = 1 to 6, are listed in table below. Table 18: Assemblage of information related to suppliers

	Supplier	Friendly level	Location	Supply ratio	Supplying (purchase amount)	Supplying price (\$/kg)	Supplying capacity (ton)	Material
	Sj		$L_{(S_j)}$	$SR_{(S_j-M)}$	$SA_{(S_j-M_i)}$	$Price_{(M_i-S_j)}$	$ASA_{(M_i-S_j)}$	$M_{i}$
<i>S</i> <sub>1</sub>	Jiatong Co.	0.3	CN	28.6%	20	56,43	50	$M_2$
<i>S</i> <sub>2</sub>	Rare-earths Co.	0.4	USA	14.3%	10	60	50	$M_2$
<i>S</i> <sub>3</sub>	Jinshu Materials	0.3	CN	57.1%	40	53,18	100	$M_2$
<b>S</b> <sub>3</sub>	Jinshu Materials	0.3	CN	87.5%	35	99,94	40	$M_1$
<i>S</i> <sub>4</sub>	Ruide Iron Co.	0.5	CN	12.5%	5	96,73	5	$M_1$
<i>S</i> <sub>5</sub>	Zhongjin Metals Co.	/	CN	0	0	0	200	$M_2$
<b>S</b> <sub>6</sub>	Iron Passion Co.	/	AU	0	0	0	150	$M_2$

## **Geographical profile**

According to above supply profile, the current supplying countries are: China (CN), and United States (US). The supplying mass and ratio from each country were calculated from supply profile and stated in the table below.

Table 19: Materials supplying amount and ratio in corresponding to supplying countries (based on the data from "Supply profile")

Materials supplying ratio & countries	CN	US
M <sub>1</sub>	100%	0%
M <sub>2</sub>	86%	14%

After the supplying countries being determined, data were collected for following impact parameters: diplomatic relation between each supplying country and France, bilateral economic exchange between each supplying country and France, and stability / ease doing business score of each supplying country. The standards for diplomatic relation are listed in methodology chapter. As the fact that France is having a comprehensive strategic partnership with China (French Ministry of foreign affairs and international development, 2013) and a strategic partnership with the United States (Juppé & Paal, 2011), a mark of 0.5 was given to

FR-CN and FR-US. Bilateral economic exchange is a sum of 1) export of France to supplying country, 2) import of France to supplying country, 3) tourist income from supplying country, 4) stock investment of France in the supplying country, 5) stock investment of the supplying country in France and 6) turnover of French companies in the country (French Gov., 2015a). In this application, the general score of stability / ease doing business is an average from following indicators: ease of doing business (The World Bank, 2016), fragile states index (FFP, 2015), estimated political stability by country (Quandl, 2015) and worldwide governance indicator (Worldbank, 2014). The data of above indicators were firstly arranged in the same order. Then they were treated to be in the same scale. Details of data treatment were stated in the methodology chapter. At the end, the average of these indicators is used to represent the result.

Table 20: Diplomatic relation, bilateral economic exchange between company located country and its supplying countries as well as the stability general score of each supplying country CN(French Gov., 2015a) US(French Gov., 2015b)

	Unit	CN	US
CL & $L_{(S_j)}$ Diplomatic relation : France &	/	0,5	0,5
$CL \And L_{(S_j)}$ Bilateral economic exchange : France &	M€	124 757	475 224
Stability / ease doing business general score of $\mathbf{L}_{(S_j)}$	/	50,3	37,0
Export of France / M€	M€	14 740	26 921
Import of France/ M€	M€	40 830	32 642
Tourist / M€	M€	684	2 047
Stock investment of France in the country / M€	M€	18 312	150 586
Stock investment of the country in France / M€	M€	1 123	62 548
Turnover of French companies in the country / M€	M€	49 068	200 480
Total	M€	124 757	475 224

Stability or ease doing business general score's evaluation method is stated below. It contains four indicators (more details are available in the methodology chapter): Ease of doing business, Fragile states index, Estimated political stability by country and Worldwide Governance Indicator.

## **Data treatment:**

In order to make the data comparable, we need to make the order of the value of each indicator reflects the same physical meaning. I.E. When the value decreases, the condition becomes better. And they are enlarged or shorten into the same scale: 0 -100.

a. For "Ease of doing business", the original values are already sorted in the determined order. So we just need to make them be scaled from 0 to 100.

China: 
$$91 \times \left(\frac{100}{189}\right) = 48.1$$
  
US:  $4 \times \left(\frac{100}{189}\right) = 2.1$ 

b. For "Fragile States Index", the original values are already sorted in the determined order. So we just need to make them be scaled from 0 to 100.

China: 
$$\left(\frac{80.9}{12}\right) - 1 \times \left(\frac{100}{9}\right) = 63.8$$
  
US:  $\left(\frac{33.5}{12}\right) - 1 \times \left(\frac{100}{9}\right) = 19.9$ 

c. For "Estimated political stability by country" indicator, the countries are scored from 2.5 (worst) to 2.5 (best). To make the value represents the determined order previously, we need to do the below calculations:

China: 
$$-(-0.54) = 0.54$$
  
US:  $-(0.63) = -0.63$ 

Then we need to make the value be scaled from 0 to 100.

China: 
$$(0.54 + 2.5) \times 20 = 60.8$$
  
US:  $(-0.63 + 2.5) \times 20 = 37.4$ 

d. For "Worldwide Governance Indicator", the countries are scored from 0 (worst) to 100 (best). So to make the value represents the determined order, we need to do the following calculations:

China: 
$$100 - 35.9 = 64.1$$
  
US:  $100 - 83.8 = 16.2$ 

The values have already been scaled from 0 to 100.

China: 64.1

US: 16.2

Table 21: Integration of Ease of doing business index and instability of supplying countries

	China 2013			US 2013			
Ease of doing business	Original Score 91	Determined order 91	0-100 scale 48.1	Original score 4	Determine order 4	ed	0-100 scale 2.1
(1 (0189)) Fragile States index (10 to 120) (FFP, 2013)	80.9	80.9	63.8	33.5	33.5		19.9
Estimated political stability by country (from $-2.5$ to $2.5$ )	-0.54	-0.54	60.8	0.63	-0.63		37.4
Worldwide Governance Indicator (from 0 to 100)	35.9	64.1	64.1	83.8	16.2		16.2
General score		China	59.2			US	18.9

#### Legislative profile

Table 22: legislation ban or hinder level	
Materials	Legislation ban or hinder level
Iron	0
Neodymium	0

In this hypothetical case, both iron and neodymium do not face a legislation (laws, directive etc.) ban or hinder the usage of this material in the permanent sector in France (Europe for his clients) in a known time.

## 2.3 Criteria calculation

### Criterion 1: Imbalance between demand & supply

The imbalance between demand and supply of  $M_i$  is the ratio of  $\frac{D_{(M_i)}}{S_{(M_i)}}$ , in which the value of demand  $D_{(M_i)}$  is in Table 12 and the value of  $S_{(M_i)}$  is the sum of ASA<sub>(M\_i-S\_i)</sub> from Table 18.

For example, the demand of  $M_1$  (neodymium) is 40 tons (table12). Its possible supply amount  $S_{(M_1)}$  can be calculated from the data in Table 18. ASA means available supplying amount (input is Table 18)  $S_{(M_1)} = \sum_{j=1}^{j=6} ASA_{(M_1 - S_j)}$   $= ASA_{(M_1 - S_4)} + ASA_{(M_1 - S_4)}$ 

$$= ASA_{(M_1-S_3)} + ASA_{(M_1-S_4)}$$
$$= 40 \text{ tons}$$
$$= 40 \text{ tons}$$

Hence, the imbalance between demand and supply of  $M_1$  is:

$$\frac{D_{(M_1)}}{S_{(M_1)}} = \frac{40 \text{ tons}}{45 \text{ tons}} = 0.889$$

In the same manner, the imbalance between demand and supply of  $M_2$  is 0.127.

## Criterion 2: Value (functional and economic) of this material to the target product

Value is the product of functional value (FV) and economic influence (EI). Its calculation formula is as below:

$$V_{(M_i)} = FV_{(M_i)} \times (EI_{(M_i)}/\$)$$

Functional value of each material  $FV_{(M_i)}$  is listed in the technical profile. The Economic influence can be calculated from the inputs of supply profile from Table 18 with following formula.

$$EI_{(M_i)} = \sum_{j=1}^{X} \left[ SA_{(M_i - S_j)} \times Price_{(M_i - S_j)} \right]$$

For example, the average of functionality value of  $M_1$  (neodymium) is 1.22 (technical profile). From Table 18, we learned that its suppliers is  $S_3$ , and  $S_4$ . So,

$$EI_{(M_1)} = \sum_{j=1}^{24} \left[ SA_{(M_1 - S_j)} \times Price_{(M_1 - S_j)} \right] = SA_{(M_1 - S_3)} \times Price_{(M_1 - S_3)} + SA_{(M_1 - S_4)} \times Price_{(M_1 - S_4)}$$
$$= 35 \text{ tons} \times 99.94 \left(\frac{\$}{\text{kg}}\right) + 5 \text{ tons} \times 96.74 \left(\frac{\$}{\text{kg}}\right)$$
$$= 3\,981\,600\,\$$$

The value of  $M_1$  is then

$$V_{(M_1)} = FV_{(M_1)} \times (\frac{EI_{(M_1)}}{\$})$$
  
= 1.22 × 3 981 600  
= 4 857 522

In the same manner, the value of  $M_2$  is 2 274 922.

## **Criterion 3: Substitutability**

As stated in the methodology chapter, substitutability was the comparison result between actual material (as reference material  $M_i$ ) and its substitute candidates ( $Stt_k$ ) in terms of functionality, technology maturity, economic aspect and resource depletion (Figure 23). Technical profile was then used to offer the functionality items as well as their weightings (Table 15). For the sake of better explanation, calculation of substitutability of  $M_1$  (neodymium) was illustrated in Table 23. In terms of functionality, the first step is to designate the functionally eligible substitute. For example, we can see that the threshold of  $F_1$  (physical carrier) is S – solid (see cell D6 of Table 23). The measurement value of neodymium ( $MV_{M_1}$ ) of  $F_1$  is also S (see cell F6 of Table 23). Measurement values of substitute candidates ( $MV_{Stt_1}$ ,  $MV_{Stt_2}$ ,  $MV_{Stt_3}$ ) under  $F_1$  are also S (see cell H6, J6, and L6 of Table 23). Threshold of  $F_4$  (maximum service temperature) is 100 °C which means the maximum service temperature of materials should be more than 100 °C in order to satisfy this functionality. We can also see from Table 23 (cells F10, H10, J10, and L10) that both reference material and substitute candidates' measurement values are higher than the

corresponding threshold. Eligible substitute is represented by 1 (when all the "functionality satisfaction with weighting of one detailed function" are positive) or 0 (when there is at least one negative "functionality satisfaction with weighting of one detailed function") (see line 20 of Table 23).



Figure 23: Substitutability evaluation mechanism in permanent magnet application

1	A	В	С	D	E	F	G	Н	I	J	К	L	М
1						Reference -	Actual product			Substitute candidates			
2						Neodymium (Nd)		Praseodymium (Pr)		Samarium (Sm)		Mixed Rai	re Earth (MRE)
3		Neodymium (Nd)	Weight	Threshold	Threshold unit	Nd2Fe14B	Functionality satisfaction with weighting	Pr2Fe14B	Functionality satisfaction with weighting	Sm2Fe14B	Functionality satisfaction with weighting	MRE-Fe-B	Functionality satisfaction with weighting
4	$F_l$	$F_l$ paraphrase	$W_{F_l}$	$Thh_{F_l}$		$MV_{M_1}$	$FSW_{(F_l-M_1)}$	$MV_{Stt_1}$	$FSW_{(F_l-Stt_1)}$	$MV_{Stt_2}$	$FSW_{(F_l-Stt_2)}$	$MV_{Stt_3}$	$FSW_{(F_l-Stt_3)}$
5	GF1	Physical Properties / Functionality	0,01		EXP()		1,59		0,02		0,02		0,02
6	F1	Physical carrier	1	S	Solid	S	100%	S	100%	S	100%	S	100%
7	F2	Hardness	0,1	80	Hv	100	3%	250	21%	200	15%	500	53%
8	F3	Density	0,6	7	g/cm3	7,4	3%	7,47	4%	7,5	4%	7,2	2%
9	GF2	Thermal Properties / Functionality	0,8		EXP()		1,49		6,30		3,96		1,78
10	F4	Maximum service temperature	0,8	100	°C	150	40%	358	206%	300	160%	200	80%
11	GF3	Magnetic Properties / Functionality	1		EXP()		11,27		1,12		12,66		1,32
12	F5	Curie temperature	1	450	°C	583	30%	564	25%	570	27%	250	-44%
13	F6	Maximum energy product (BH) max	1	70	kJ/m3	289	313%	73,9	6%	300	329%	150	114%
14	F7	Residual Induction Br	1	1,15	T	1,31	14%	1,18	3%	1,1	-4%	1,18	3%
15	F8	Residual magnetic flux density	0,8	1,15	Bt/T	1,23	6%	1,35	14%	1,38	16%	1,19	3%
16	F9	Coecitivity	1	200	KA/m (HcB)	880	340%	211,4	6%	900	350%	150	-25%
17		Total functionality satisfaction			EXP()	1	2,48		7,43	1	6,63		3,12
18		Individual functionality NOT satisfy the threshold Nb					0		0		1		2
19		Average functionality satisfaction among the functionalities which satisfy the threshold			%	9	94%		43%	125%		51%	
20		Eligible substitutes					1 1		1	0		0	
21	*	Relative functionality satisfaction benchmarking (FRS)	1			1	00%	60%		133%		25%	
22	*	Technology maturity of producing (TM)	1			1	00%		80%	7	/5%		60%
23		Price of materials (metal, not oxide) (21 dec 2014)			\$/kg	8	7,00	1	75,00	20	0,00	2	.9,80
24		Mass needed compared to reference - 1kg of Nd			kg	1	.,00		0,98	1	.,04		J,97
25		Cost benchmarking with a reference of 1 kg of Nd			\$	8	7,00	1	70,98	20	0,84	2	.9,00
26		Cost difference between reference and substitutes				(	),00	-	0,97	C	),76		J,67
27	*	Economic acceptability of eligible substitutes (EA)	1		EXP()	1	00%		38%	2	14%	1	195%
28		Resource depletion ratio of material (ecoinvent)				3	3,50		3,60	5	5,20		2,00
29		Resource depletion ratio benchmarking with the reference				(	),00	-	0,03	-(	),49		),43
30		Resource depletion between reference and substitutes			EXP()	1	.,00		0,97	C	),62		1,54
31	*	Resource depletion benchmarking (RDB)	1			1	00%		97%	6	52%	1	154%
32 General evaluation of substituting performance						1	00%		69%	1	21%	1	108%
33		Substitutability of Neodymium (Nd)						69%					
1	A	В	С	D	E	F	G	Н	I	J	К	L	Μ

## Table 23: Substitutability evaluation of neodymium in permanent magnet application (figures in orange mean they are imaged)
The second step is to calculate the substitutability satisfaction with weighting (see colon G, I, K, and M of Table 23). If we take  $GF_2$  as example, it contains only one functionality  $F_4$ . The substitutability satisfaction of  $Stt_1$  (praseodymium) under  $F_4$  with weighting is:

$$FSW_{(F_4 - Stt_1)} = \left| \frac{MV_{(F_4 - Stt_1)} - Thh_{F_4}}{Thh_{F_4}} \right| \times W_{F_4}$$
$$= \left| \frac{358 - 100}{100} \right| \times 0.8 = 206\%$$

Then it is to calculate the General functionality (GF)'s FSW value:

$$FSW_{(GF_2-Stt_1)} = \overline{e^{FSW_{(F_4-Stt_1)}}} \times W_{GF_2} = e^{206\%} \times 0.8 = 7.88 \times 0.8 = 6.30$$

In the same manner, we can obtain the  $FSW_{(GF_1-Stt_1)}$  and  $FSW_{(GF_3-Stt_1)}$  as below:

$$FSW_{(GF_1 - Stt_1)} = \left(\overline{e^{FSW_{(F_1 - Stt_1)}} + e^{FSW_{(F_2 - Stt_1)}} + e^{FSW_{(F_3 - Stt_1)}}}\right) \times W_{GF_1}$$
$$= \left(\overline{e^{100\%} + e^{21\%} + e^{4\%}}\right) \times 0.01 = 0.02$$

$$FSW_{(GF_3 - Stt_1)} = \left( e^{FSW_{(F_5 - Stt_1)}} + e^{FSW_{(F_6 - Stt_1)}} + e^{FSW_{(F_7 - Stt_1)}} + e^{FSW_{(F_8 - Stt_1)}} + e^{FSW_{(F_9 - Stt_1)}} \right) \\ \times W_{GF_3} = \left( \overline{e^{25\%} + e^{6\%} + e^{3\%} + e^{14\%} + e^{6\%}} \right) \times 1 = 1.12$$

The third step is to calculate total functionality satisfaction of the eligible substitute (line 21 of Table 23). If we take  $Stt_1$  as example,

$$FSW_{(Stt_1)} = \sum_{L=1}^{3} FSW_{(GF_L - Stt_1)} = FSW_{(GF_1 - Stt_1)} + FSW_{(GF_2 - Stt_1)} + FSW_{(GF_3 - Stt_1)} = 0.02 + 6.30 + 1.12 = 7.43$$

In the same manner, we obtain the  $FSW_{(M_1)} = 12.48$ 

Then Relative Functionality Satisfaction (RFS) benchmarking of praseodymium is calculated as below. Its result is represented in line 21 of Table 23.

$$RFS_{Stt_1} = \frac{FSW_{Stt_1}}{FSW_{M_1}} = \frac{7.43}{12.48} = 60\%$$

In terms of technology maturity of producing, it is determined subjectively in this application (see line 22 of Table 23).

In terms of economic, we firstly need to calculate  $C_{Stt_1}$ , cost of substitute with equivalent of 1 kg of reference material  $M_i$  with equation below. Its results are in line 25 of Table 23.

$$C_{Stt_1} = M2R_{Stt_1} * PoM_{Stt_1} = 0.98 \ kg \times 175 \frac{\$}{kg} = 170.98 \ \$$$

With

 $M2R_{Stt_1}$ : Mass of 1<sup>st</sup> substitute (praseodymium) needed compared to 1 kg of reference material (neodymium) = 0.98 kg (cell H:I 24 pf Table 23)

 $PoM_{Stt_1}$ : Price of material  $Stt_1$  (praseodymium) per kg = 175 \$/kg (cell H:I 23 of Table 23).

 $CD_{Stt_1}$ , Cost difference (CD) between praseodymium and reference material  $M_1$  is calculated as below. The result of cost difference is represented in line 26 of Table 23.

$$CD_{Stt_1} = \frac{C_{M_1} - C_{Stt_1}}{C_{M_1}} = \frac{87 - 175}{87} = -0.97$$

With

 $C_{M_1}$ : cost of 1 kg of  $M_1$  = price of  $M_1$  = 87 \$/ kg. (line 23 of Table 9).

Finally, economic acceptability of substitute – praseodymium is calculated as below. Its results are represented in line 27 of Table 23.

$$EA_{Stt_1} = e^{CD_{Stt_1}} = e^{-0.97} = 38\%$$

In terms of resource depletion, the resource depletion ratio of these materials from database Eco invent (see line 28 of Table 23) was input directly, from what we can calculate *RDRBR*: Resource depletion ratio benchmarking with the reference material as equation below.

$$RDRBR_{Stt_1} = \frac{RDR_{M_1} - RDR_{Stt_1}}{RDR_{M_1}} = \frac{3.50 - 3.60}{3.50} = -0.03$$

With

 $RDR_{M_1}$ : Resource depletion ratio of  $M_1 = 3.50$  (cell F: G 28)

 $RDR_{Stt_1}$ : Resource depletion ratio of  $Stt_1 = 3.60$  (cell H: I 28)

Then, we need to use *RDRBR*'s exponential function value to solve the negative or positive problem according to the following formula. Its result is represented in line 31 of Table 23.

$$Exp(RDRBR_{Stt_1}) = e^{RDRBR_{Stt_1}} = e^{-0.03} = 97\%$$

By combining the above four terms (marque with \* in colon A), we can obtain the General Evaluation of Substitute's Performance of  $Stt_1(GESP_{Stt_1})$  as below. Its results are represented in line 32 of Table 23.

$$GESP_{Stt_1} = \overline{\left(RFS_{Stt_1} + TM_{Stt_1} + EA_{Stt_1} + RDB_{Stt_1}\right)} = \overline{\left(60\% + 80\% + 38\% + 97\%\right)} = 69\%$$

As only praseodymium is designated as eligible, the substitutability of  $M_1$  after considering all substitutes can be obtained from formula below.

$$Substitutability_{Stt_1} = \sum_{k=1}^{3} (GESP_{Stt_k}) \times Egibility = GESP_{Stt_1} \times 1 = 69\%$$

In the same manner, the substitutability of iron is 48%. As the fact that we need them in the right order which means when values of each criterion increases, it contributes more to the criticality. For this criterion, the reciprocal of above values were used for final criticality evaluation. Hence,

Right order of Substitutability<sub>Stt1</sub> = 
$$\frac{1}{69\%}$$
 = 1.45  
Right order of Substitutability<sub>Stt2</sub> =  $\frac{1}{48\%}$  = 2.08

### **Criterion 4: Environmental friendly level**

From Eco-invent, we obtained the human toxicity with a unit of kg 1,4-DCB-Eq /1kg of material (Table 13). The environmental friendly level of one material is equal to the selected indicator multiplied by its mass.

For example, human toxicity value of  $M_1$  (neodymium) is 709.96 kg 1,4-DCB-Eq /1kg of  $M_1$  while its demand amount is 40 tons. Hence, its environmental friendly level is:

Environmental friendly 
$$level_{(M_1)}$$
  
=  $D_{(M_1)}$  × selected environmental indicator  
= (40 000 kg of  $M_1$ ) ×  $\frac{709.96 \text{ kg } 1.4 - \text{DCB} - \text{Eq}}{1 \text{ kg of } M_1}$   
= 28 398 400 kg of 1.4 - DCB - Eq

In the same manner, *Environmental friendly level\_{(M\_2)}* is 40 392 800 000 kg of 1,4 – DCB – Eq.

### **Criterion 5: Legislation ban or hinder level**

In this hypothetical application, both iron and neodymium do not face a legislation (laws, directive etc.) ban or hinder the usage of this material in the permanent sector in France (Europe for his clients) in a known time.

### **Criterion 6: Quality of relationship with suppliers**

The relationship with suppliers is marked with following five factors: quality of supplying materials, timeliness, innovation, exchange and human. These scores were obtained randomly. Their general scores were represented in Table 18 of supply profile. The quality of relationship is the product of general relationship score and the supplying share with below formula. For example,  $M_1$  has following suppliers:  $S_3$  and  $S_4$ . Their supplying shares are:  $SR_{(S_3-M_1)} = 87.5\%$ ,  $SR_{(S_4-M_1)} = 12.5\%$ . The qualities of relationship with these suppliers (QRS) are:  $QRS_{S_3} = 0.3$ , and  $QRS_{S_4} = 0.5$ ,. Hence, the quality of relationship with the suppliers of  $M_1$  is:

$$QRS_{M_1} = \sum_{j=1}^{6} SR_{(S_j - M_1)}^2 \times QRS_{S_j}, j = 3, 4$$
$$= 87.5\%^2 \times 0.3 + 12.5\%^2 \times 0.5$$
$$= 0.24$$

In the same manner,  $QRS_{M_2}$  is 0.13

## **Criterion 7: Depletion of reserves**

With data in the material profile (see Table 12), depletion of reserves is calculated as below.

$$DoR_{M_{1}} = \frac{Global \ production \ amount \ of \ neodymium}{Global \ reserve \ amount \ of \ neodymium}$$
$$= \frac{GProd_{M_{1}}}{GRsv_{M_{1}}}$$
$$= \frac{0.11 \ million \ tons}{140 \ million \ tons}$$
$$= 0,000786$$

In the same manner,  $DoR_{M_2}$  is 0.018258

# **Criterion 8: Geo-relation (political and bilateral economic exchange) between supplying and buying countries**

This criterion needs the input from supplier profile and geographic profile. For example,  $M_1$  (neodymium) has suppliers of  $S_3$  and  $S_4$ .  $L_{(S_3)} = L_{(S_4)} = CN$  which means these suppliers are both from China.  $SR_{(S_3-M_1)} = 87.5\%$  and  $SR_{(S_4-M_1)} = 12.5\%$  which means supplying ratio of  $S_3$  to  $M_1$  is 87.5% and supplying ratio of  $S_4$  to  $M_1$  is 12.5% (Table 18). The diplomatic score between the company located country CL (France) and their supplying county (CN) is given a score of 0.5 (see geographical profile Table 20). The bilateral economic exchange amounts between the company located country (France) and the supplying country China is 124 757 million euros.

Based on the equation below, we have:

$$\begin{split} & Geo-relation_{M_{1}} = \frac{Diplomatic\ score_{M_{11}}}{Economic\ bilateral\ exchange\ (M \in)_{M_{1}}} \\ &= \frac{\sum_{j=1}^{6}(SR_{(S_{j}-M_{1})} \times Diplomatic\ score_{CL-L_{(S_{j})}})}{\sum_{j=1}^{6}(SR_{(S_{j}-M_{1})} \times Economic\ bilateral\ exchange_{CL-L_{(S_{j})}})} \\ &= \frac{SR_{(S_{3}-M_{1})} \times Dipl.\ sco_{CL-L_{(S_{3})}} + SR_{(S_{4}-M_{1})} \times Dip.\ sco_{CL-L_{(S_{4})}}}{SR_{(S_{3}-M_{1})} \times Eco.\ bil.\ exc._{CL-L_{(S_{3})}} + SR_{(S_{4}-M_{1})} \times Eco.\ bil.\ exc._{CL-L_{(S_{j})}}} \\ &= \frac{87.5\% \times 0.5 + 12.5\% \times 0.5}{87.5\% \times 124\ 757 + 12.5\% \times 124\ 757} = 0.0000040 \end{split}$$

In the same manner,  $Geo - relation_{M_2}$  is 0.0000028

## **Criterion 9: Global demand to supply ratio**

Alonso et al. (2012) developed an evaluation methodology of demand and supply ratio of REE. They also stated the methods and different scenarios to forecast the demand and supply. As stated in methodology chapter, we can use directly the results or methods developed by other researcher in this criticality evaluation, hence demand supply ratio of neodymium is based from Alonso's study: 106% for 2010 and 724% for 2035.

For iron, the demand amount of iron in 2011 was around 190 million tons (Burns, 2011) and the supply amount is 340 million tons (Fast FT, 2015). Hence, demand supply ratio of iron is

demand supply ratio<sub>iron</sub> = 
$$\frac{demand \ amount_{iron}}{supply \ amount_{iron}} = \frac{190}{340} = 56\%$$

## **Criterion 10: Stability of supplying country**

Let us still take  $M_1$  as example. Its suppliers' information is stated above. The stabilities of its supplying countries China is 59.2 (see Table 21). Hence the stability of supplying countries of  $M_1$  is as below.

Stability of supplying country<sub>M1</sub> =  
= 
$$\sum_{j=1}^{6} (SR_{(S_j - M_1)} \times Stability general score_{L_{(S_j)}})$$
  
= 86% × 59.2 + 14% × 59.2 = 59.2

In the same manner, the *Stability of supplying country*<sub> $M_2$ </sub> is 53.5.

If we applied the same formula to calculate the stability in the European Commission's criticality study, then the stability of supplying countries of  $M_{10}$  is as below.

Stability of supplying country<sub>M1</sub> =  
= 
$$\sum_{k=1}^{6} (SR_{(S_{k-M})}^{2} \times Stability general score_{L_{k}})^{2}$$

$$= \sum_{j=1}^{\infty} (SR_{(S_j - M_1)}^2 \times Stability \text{ general score }_{L_{(S_j)}})$$
  
= 87.5%<sup>2</sup> × 59.2 + 12.5%<sup>2</sup> × 59.2 = 46.25

## **Criterion 11: Recycling rate**

The contribution of recycling rate to the criticality is calculated as below:

$$1 - Recycling rate_{M_i}$$

The end of life recycling rate of each material is showed in Table 1. Recycling  $rate_{M_1} = 1\%$ and Recycling  $rate_{M_2} = 75\%$ , which means contribution of recycling rate of  $M_1$  is:

$$1 - Recycling rate_{M_1} = 1 - 1\% = 0.99$$

In the same manner,  $M_2$  has a score of 0.25 for this criterion.

## 3. Results

## 3.1 Results presentation

Table 24: Assemblage of criteria's calculation results (threshold values – figures in orange were determined by author subjectively)

			Co Right o	lon A rder value	Co (value-	olon B thre.)/thre.	Colon C e^ exponentian function		
	Sub-Criterion	Thre.	$M_1$ (Nd)	<i>M</i> <sub>2</sub> (Fe)	$M_1$ (Nd)	$M_2$ (Fe)	$M_1$ (Nd)	$M_2$ (Fe)	Thre.
1	Imbalance demand&supply	0,6	0,889	0,127	0,482	-0,788	1,619	0,455	1
2	Value	3 000 000	4 857 552	2 274 922	0,619	-0,242	1,857	0,785	1
3	Substitutability	1,3	1,45	2,08	0,115	0,600	1,122	1,822	1
4	Environment friendly level	3000000000	28398400	40392800000	-0,999	0,346	0,368	1,414	1
5	Legislation ban or hinder level	0	0	0	0	0	1,000	1,000	1
6	Quanlity of relationship with suppliers	0,5	0,24	0,13	-0,520	-0,740	0,595	0,477	1
7	Depletion of reserves (prod/reserve)	0,05	0,000786	0,018258	-0,984	-0,635	0,374	0,530	1
8	Geo relation (politic + economic)	0,0000035	0.0000040	0.0000028	0,143	-0,200	1,154	0,819	1
9	Global demand supply ratio	1	1,06	0,56	0,060	-0,440	1,062	0,644	1
10	Stability of suppmying country	70	59,2	53,4	-0,154	-0,236	0,857	0,790	1
11	Recycling rate	0,5	0,99	0,28	0,980	-0,440	2,664	0,644	1
		12,7	9,4						

Calculation results of above selected criteria are represented in the colon A of above table. The first step of data treatment is to put them in the right order which means when the value of each criterion increase, it contributes more to the criticality. This step is conducted during the criteria calculation in this application. The second step is to calculate the relative value of each criterion based on corresponding threshold (see colon B). The third step is to use exponential function to eliminate negative values and make them in the same baseline (see colon C). General criticality score of  $M_1$  (neodymium) is 12.7 and 9.3 for  $M_2$  (iron) which means neodymium is more critical in general than iron in this application. The results are also illustrated in the radar chart below.



Figure 24: Radar charts of criticality of materials Neodymium and Iron for permanent magnet application

The pink area in above figure represents the criticality of neodymium while the blue represents the iron. Their areas' sizes also show their general criticality score. Red circle in the figure shows the threshold. Each criterion corresponds to one horn of the color areas in the figure. When one horn of an area surpasses the red circle, it means its value is worrisome and needs attention. For example, recycling rate of neodymium is the horn which surpassed red circle the most. It means recycling rate of neodymium contributed the most to its criticality and deserves more attention than other criteria for neodymium. If both materials remain inside the red circle for one criterion, such as depletion of reserves, it means they did not contribute too much to the criticality and we do not need to worry about the reserve depletion of these materials. From the radar figure, we can more intuitively tell which material is more critical and which criteria made them critical. It is also a guideline of priority for searching solutions.

## 3.2 Completeness of study

## **Coverage of impact parameters**

Being combined with Figure 8 – "Impact parameters (IP) from the diagnosis part" of chapter 3, this section shows the coverage of impact parameters in this application. If we assume that all indicators' evaluation methods and inputs are accurate, more impact parameters being covered means that the study is more comprehensive and credible. Results of coverage analysis are represented in the figure below. Black solid IP block means it is covered. While IP block means it is not considered in the study. Color depth of block represents the completeness of corresponding item. Part "a" of Figure 25 shows the coverage of impact parameters in the dimension of importance. As all the impact parameters were considered in the study, its coverage is 100%.



Figure 25 (a): Coverage of impact parameters in the dimension of Importance in permanent magnet application



Figure 25 (b): Coverage of impact parameters in the dimension of Imbalance demand & supply in permanent magnet application

Part "b" of Figure 25 shows that 50% of impact parameters were considered in the dimension of imbalance between demand and supply. We can see the "demand" block contains IP 38 and IP 6 blocks so that IP38 and IP6 both has a weight of  $\frac{1}{2}$ . Block IP 6 is solid black and IP38 block is white so that the completeness of "demand" block is  $\frac{1}{2} \times 1 + \frac{1}{2} \times 0 = 50\%$ . In the same manner, we can obtain the completeness of "supply" block which is also 50%. As this dimension contains two branches (demand and supply), each branch has a weight of  $\frac{1}{2}$ . The completeness of "Imbalance between demand and supply" is 50%. Part "c" of Figure 25 shows that the completeness of dimension of accessibility is 83%.

As this application is based on basic model, above coverage analysis also corresponds to the situation of how many impact parameters listed in diagnosis chapter were covered in basic model.



Figure 25 (c): Coverage of impact parameters in the dimension of accessibility

## **CHAPTER 6**

## Part II AN APPLICATION ON LIGHT EMITTING DIODE

## 1. Introduction

Light emitting diode (LED) is a lighting technology discovered in the early 20<sup>th</sup> century which can emit light from a solid-state material at room temperature. Due to its high energy efficiency and long lasting life, LED has been regarded as the most promising technology which can replace the conventional lightings in the future. MacKinsey (2012) predicted that LED will make up almost 70% of general lighting market in 2020 while there was only less than 1% of LED in 2008 and 13% in 2012 in the United Kingdom (Navigant Consulting Europe, 2009). This lighting transition will also lead the demand increase of corresponding materials. This potential enormous increase of demand has drawn our interest to know which materials are more critical and deserve more attention in advance. White LED is the common lamp for general housing lighting. There are three technologies to generate white light for LEDs: phosphor converting, color mixing and hybrid method. The blue-light emitting phosphor converting LED is the most widely used to generate white light (Scholand & Dillon, 2012). That's why a white LED which is based on blue-light emitting converted by yellow phosphor is selected as the theoretical application subject to demonstrate how to apply the "Materials Criticality Profiling Methodology (MCPM)".

The structure of chapter is similar to previous application: Firstly, scenario and basic information for this application is introduced. Secondly, data collections based on material, technical, supplier and geographical related profiles are illustrated. Thirdly, calculation is demonstrated with one example for each criterion. Finally, the general score of criticality is presented with a histogram. Results are also divided into three groups and showed in radar charts according to their criticality levels. Sensitivity analysis and completeness of this application are stated. It ends with the discussion of limitations from this application and observations.

## 2. Scenario and data collection

## 2.1 Scope and scenario

In this application, I assumed that a French lighting company is producing a similar product as the Philips Endurant LED lamp. The company is located in France which makes CL = France. The research subject *P* is the LEDs (not the whole lamp) contained inside. The time scale of data is around 2012.

To simplify the scenario and reduce the number of materials to be analyzed, the materials candidates are selected if they contain metal elements. The LED structure as well as materials for each part is as following: Quantum Wells (QWS) & n-p players (TMGa, TMIn, TMAl), metal contacts (Al, Ni, Ag, Ti, W), sapphire substrate (Alumina), solder layer (AuSn solder), sub mount (Alumina), phosphor (Ce3+:YAG) and wire bond (gold). In this study, the difference between alumina of sapphire substrate (to grow QWS) and the one of sub mount (to support semiconductor) is ignored. The mass of alumina purchased to produce sapphire substrate (level 2 of Figure 26) is more than 100 times of sub mount's. In total, there are 12 materials to be analyzed in this study, where N = 12. Their detailed names are as below with each one being given a code  $M_i$ , *i* is from 1 to 12.

$M_1 = \text{Ce } 3 + : \text{YAG}$	$M_5 = Al$	$M_{10} = Alumina$
(Y3Al5012(Ce))	$M_6 = Ni$	$M_{11} = AuSn \ solder$
$M_2 = TMGa (Ga(CH3)3)$	$M_7 = Ag$	$M_{12} = Gold$
$M_3 = TMIn (InC3H9)$	$M_8 = Ti$	
$M_4 = TMAl \ (C6H18Al2)$	$M_9 = W$	



Figure 26: Stratification of data of materials consumption for producing LED in this application

The materials flow has been retrospect to raw materials and ends with study subject (product). Materials are classified into three levels (Figure 26). The materials (components or elements) contained inside the study subject are classified as level 3. In order to produce the product, materials purchased for the manufacturing or assemblage (depends on the study scope) are level 2. Raw materials used to produce the level 2 materials are classified as level 1. The European Commission's (2010, 2014) critical materials studies are based on the level 1. Between level 2 and 1, there can be intermediates but they are ignored in order to reduce complexity. From the figure above, we can also tell that Materials Flow Analysis (MFA) can assist the criticality study by offering a clear view of related materials as well as their exact flow data.

In this application, materials candidates were selected from level 2 (purchased materials for manufacturing) due to data availability. The following data are also related to level 2: supplier, functionality and substitutability. The level 3 (elements contained in a finished LED) materials were then reckoned from level 2. Then the corresponding metals are considered as level 1. For example, the LED's QWS contains Ga element (level 3). It is made from TMGa (level 2) which is also the materials that Company purchased for manufacturing. If we retrospect more, one of raw materials to make TMGa is gallium mineral (level 1). In this study, I only took account of direct related raw mineral materials which excludes the energy

materials, water, dimethylzinc, etc. even they were required for producing TMGa. And the retrospect stops to metal or metallic oxide status (gallium metal) instead of zinc ores or bauxites. The production loss between level 1 and 2 material is not taken into account neither. The following data are related to level 1: global reserve, resource, production amount, global demand and supply amount, recycling rate, environmental and regulative inputs. The amount of raw materials used to produce the same element but with different physical or chemical structure as well as functions might be different. For instance, the raw materials information to produce Al in QWS inside LED is not exactly the same with the Al of metal contact in terms of materials types and amount. However, I assumed that they are equivalent in terms of metals and the difference of the raw materials to produce those metals is not taken into account here.

The scenario selected is the basic one which is stated in the methodology chapter and illustrated in the permanent magnet application. After scenario type is chosen, the impact parameters and calculation model is determined as well.

## 2.2 Data collection

### Materials profile to produce one LED

In order to produce one LED, the amount of selected materials to be purchased is 1,59068 g (based on calculations of data from the DOE report (Scholand & Dillon, 2012)). Mass ratio of each material  $R_{(M_i)}$  is showed in Table 25, as well as their mass amounts.

Based on the Mckinsey (2012) report, there are 283 million pieces (73 m pcs of retrofit LED and 210 m pcs of full LED) of LED in 2012 and 3 285 million pcs (264 m pcs of retrofit LED and 3 021 m pcs of full LED) of LED in 2020 among general lighting (residential, office, industrial, shop, hospitality, outdoor and architectural) fixtures. As the fact that LED technologies was applied for general lighting not long time ago and LED lamps have already 30 000 hours of lifetime, the replacement number of LED lamps is neglected. High power LED shares around 33% of LED revenues in 2012 and 25% of LED revenues in 2017 (View, 2014). I assume that there is 33% of high power LED in 2012. Among the LEDs, Philips occupies around 12% (Guerster, 2013) of the market share. From their current official French website (Philips Lighting, 2016), 15 types of high power LED lamps were found. Although

the Philips Endurant model was not available in this website any more, I assumed that this model made up around 7% of the Philips lamps in 2012.

$$283\ 000\ 000 \times 33\% \times 12\% \times 7\% = 784\ 476$$

From the above assumptions, the sale amount of Philips Endurant LED lamps was obtained 784 476 pieces. The demand amount as the production target was rounded to 1 million in 2012 for following reasons: 1) the 784 476 is not the real number anyway so that accuracy will not be influenced too much if we take its approximate value; 2) the approximate value – one million is easier to be operated if other researchers have more accurate number in the future. I also assume that the LED lamp of this application contains 12 LEDs as Philips Endurant LED lamp (Scholand & Dillon, 2012). Then the demand amount for this type of LED is 12 000 000 pcs in 2012. In addition to the mass ratio of each material required to produce one LED (Table 25), we can obtain the demand amount of each material  $D_{(M_i)}$  as stated in Table 25 as well.

The global reserve and production amount represent level 1 (metal as raw materials). They are equivalent to level 3 (mineral elements) in this study which means the materials loss between these two levels were ignored. The global reserve amount of its related mineral elements is the sum of reserve amount of related minerals multiplied by its corresponding ratio (more detail is available in criterion 8). Global reserve and production amount of related minerals data are based on the USGS mineral commodity summaries on (USGS, 2016). According to above methods, we can obtain the global reserve and production amount of its related mineral elements, respectively correspond to  $\text{GRsv}_{M_i}$  and  $\text{GProd}_{M_i}$ , as showed in Table 25. In like manner, the contribution of criticality in terms of recycling and environment for each material is obtained. For contribution of environmental aspect, human toxicity is used as indicator. Environmental data are from Eco invent. Recycling rate of Ag, Al, Au, Ni, Ti and Ware were calculated as recovered materials from new or old scraps divided by total mine production (USGS, 2016). Recycling rate of Ce, Ga, In and Y are from Buchert et al., (2012) and recycling rate of Sn is from Russell & Lee (2005). Above results are assembled in the table below.

### Table 25: Materials related inputs

Code	Unit	<i>i</i> = 1	<i>i</i> = 2	<i>i</i> = 3	<i>i</i> = 4	<i>i</i> = 5	i = 6	<i>i</i> = 7	<i>i</i> = 8	i = 9	<i>i</i> = 10	<i>i</i> = 11	<i>i</i> = 12
	/	<i>M</i> <sub>1</sub>	<i>M</i> <sub>2</sub>	<i>M</i> <sub>3</sub>	$M_4$	$M_5$	<i>M</i> <sub>6</sub>	<i>M</i> <sub>7</sub>	<i>M</i> <sub>8</sub>	$M_9$	<i>M</i> <sub>10</sub>	<i>M</i> <sub>11</sub>	<i>M</i> <sub>12</sub>
M <sub>i</sub>	/	Ce 3+: YAG	TMGa	TMIn	TMAl	Al	Ni	Ag	Ti	W	Alumina	AuSn	Gold
		(Y3Al5O12(Ce))	(Ga(CH3)3)	(InC3H9)	(C6H18Al2)							solder	
$\mathbf{R}_{(\mathbf{M}_i)}$	%	0,055%	7,701%	0,052%	0,016%	0,016%	0,021%	0,026%	2,462%	0,314%	87,813%	1,519%	0,004%
Mass	g	0,00087	0,12250	0,00083	0,00025	0,00025	0,00033	0,00042	0,03917	0,00500	1,39683	0,02417	0,00006
$\boldsymbol{D}_{(\boldsymbol{M}_i)}$	g	10 440	1 470 000	9 960	3 000	3 000	3 960	5 040	470 040	60 000	16 761	290 040	720
											960		
GRsv <sub>Mi</sub>	tons	1440847,6	609000	7909	23587,5	62900	8100000	520000	1120300	3300000	33274,1	1843865	55000
$GProd_{M_i}$	tons	13714,065	166,257	143,081	17850	47600	2630000	26000	209000	81400	25180,4	112582,4	2800
Human	kg 1,4-	107,0466244	1080,1224	13358,301	61,0425	162,78	2992,9	310940	0,21438	2305,9	86,11062	812,44631	1093,3
toxicity	DCB-												
	Eq /1kg												
	of												
	material												
Recycling	/	8%	0,00%	17%	17%	46%	41%	47%	24%	53%	24%	43%	32%

### **Technical profile of LED**

A functionality structure diagram is a scheme which shows the breakdown of a product's function system to its distal function that the materials inside offered. It can help well determine functionalities when a product is too complex. This kind of information is usually available in the product design department. In this application, the LED functionalities structure diagram (Figure 27) was conducted in two levels based on LED structure and components. Seven general functionalities were determined first and then refined into 15 functionalities. Hence, Z = 7,  $GF_L$ , L = 1 to 7 . H = 15,  $F_l$ , l = 1 to 15 . After the functionality structure being determined, following methods were used to give weighting. 1) Excel sheets for functionality weighting are built as well as the instructions. 2) A panel of LED experts is selected for fulfilling the previous sheets. 3) The first round weighting is executed: ask experts to fulfil the sheets with comments. 4) Collect the marks and comments from the first round. Calculate the weights and consistence of each matrix inside. And show them anonymously to every member. 5) Final round: ask the members to remark again after having reviewed the marks and comments of others. 6) Use the average of results from the final round. This weighting method is a combination of Analytical Hierarchy Process and Delphi's method.



Figure 27: Functionalities structure diagram of LED

In more details of functionality weighting, five matrixes were extracted based on the structure diagram. Experts fulfil each matrix according to standards of Table 26. For example, the matrix 1 is to determine weightings of general functionalities to LED.

#### Table 26: standards to give weighting to general functionalities to LED

aij = 1,	General functionality "i" is as same important as the General functionality "j" to LED
aij = 3,	General functionality "i" is slightly important than the General functionality "j" to LED
aij = 5,	General functionality "i" is more important than the General functionality "j" to LED
aij = 7,	General functionality "i" is much more important than the General functionality "j" to LED
aij = 9,	General functionality "i" is extreme more important than the General functionality "j" to LED

#### Table 27: Form of getting value for Matrix 1



Table above shows the form where experts fulfil the weightings with the help of standards stated previously. For example,  $a_{11} = 1$  means that GF1 is as important as GF1 which is the same for  $a_{22}$  to  $a_{77}$ . If  $a_{16} = 5$ , it means GF1 is more important than GF6. The up area is where experts fulfilled the numbers. The down area is the reciprocal of up area. I.E.  $a_{ij}$  of down area is reciprocal of  $a_{ji}$  of up area. During the calculation of weighting and consistence, Matlab tool was used. The results of weighting of functionality to LED and the functionality value (FV) of each material are showed in Figure 28 and 29 separately. From Figure 28, we can see F1 and F2 are the two most important functionalities to LED according to surveys, followed by F3, F4 and F5. The rest are relatively less important than them. The sum of these functionality weightings is equal to 1, so is the functionality value of materials. The weightings of functionalities can serve more in substitutability evaluation.



Figure 28: Weighting of each functionality to LED



Figure 29: Functionality value (FV) of each material to LED

According to surveys, the functionality values offered by TMGa, TMIn and TMAl are the most important. They are materials made up quantum wells & n-p layers which allow blue light generating inside LED. After that, it is alumina which made up of sapphire substrate. The sapphire substrate is where grow the quantum wells. Without its supporting, the light generating materials cannot be carried. Above four materials all required atomic matching and are core of LED lighting technology. It's reasonable that they were regarded as most important in terms of function.

## Supply profile

S<sub>14</sub>

*S*<sub>19</sub>

Sg

 $S_1$ 

*S*<sub>19</sub>

S<sub>9</sub>

*S*<sub>1</sub>

*S*<sub>19</sub>

Kyocera

SAFC

DOW

SAFC

DOW

SAFC

AkzoNobel

AkzoNobel

Supply profile is one of the keys to personalize each criticality study even when the subject product remains same. Different choices of suppliers lead to different supplying countries, supplying ratios, supplying capacities, supplying prices and relationship qualities between the Company and these suppliers. Above information projects the supply amount and direct supplying capacity from these suppliers. The price represents the direct cost to purchase those materials and is related to their economic influence. In addition, supplying country information represents the geographic aspect which will be explained more in next section of this chapter. This information leads to the stability of those countries as well as bilateral relation between them and the country where located the Company. If we consider impact parameters which were not taken into account in basic case, it will also relate to the inside demands in supplying countries as well as other restrictions inside supplying countries. It is one of the approaches to externalize dynamic aspect of criticality.

As I do not access the real supplier information of a LED company, three suppliers were selected randomly for each material from current available market for this hypothetical application. The total numbers of suppliers is 24 in this study which means X = 24 because some suppliers are offering more than one material. The suppliers,  $S_j$ ,  $_j = 1$  to 24, are listed in table below.

	Supplier	Location <sup>6</sup>	Supply ratio	Supplying amount	Supplying price (\$/g)	Supplying capacity (g)	Materi
	Sj	$L_{(S_j)}$	$SR_{(S_j-M_i)}$	$SA_{(S_j-M_i)}$	$Price_{(M_i-S_j)}$	$ASA_{(M_i-S_j)}$	M <sub>i</sub>
<b>S</b> <sub>8</sub>	Crystal Applied	TW	42%	7040023,2	0.6	26559936	$M_{10}$
<i>S</i> <sub>21</sub>	STA	KR	31%	5196207,6	0.6	19919952	<i>M</i> <sub>10</sub>

26%

17%

33%

50%

17%

33%

50%

17%

4358109,6

249900

485100

735000

1693.2

3286,8

4980

510

0.6

2

2

2

20

20

20

8

16599960

6800000

13200000

20000000

340000

660000

1000000

1700000

JP

US

KR

NL

US

KR

NL

US

rial

 $M_{10}$ 

 $M_2$ 

 $M_2$ 

 $M_2$ 

 $M_3$ 

 $M_3$ 

 $M_3$ 

 $M_4$ 

Table 28: Assemblage of information related to suppliers (suppliers search engines used are Alibaba, Thomasnet and google. Data are based on their product pages available in above websites and information requiring emails.)

<b>S</b> 9	DOW	KR	33%	990	8	3300000	$M_4$
<i>S</i> <sub>1</sub>	AkzoNobel	NL	50%	1500	8	500000	$M_4$
<i>S</i> <sub>24</sub>	Zhuhai Hanbo Trading	CN	33,30%	3476,52	1.25	12000000	$M_1$
<i>S</i> <sub>2</sub>	Beijing Yuji Science and Technology Co	CN	33,30%	3476,52	1.65	2500000	<i>M</i> <sub>1</sub>
<i>S</i> <sub>15</sub>	Longkou Unity Machinery Equipment Co	CN	33,30%	3476,52	3	52000000	<i>M</i> <sub>1</sub>
<i>S</i> <sub>13</sub>	Jiangsu Plaza Premium Electric Instrument	CN	33,30%	239,76	91.6	72000	<i>M</i> <sub>12</sub>
<i>S</i> <sub>3</sub>	California Fine Wire	US	33,30%	239,76	91.6	72000	<i>M</i> <sub>12</sub>
<i>S</i> <sub>10</sub>	Haraeus	GM	33,30%	239,76	91.6	72000	<i>M</i> <sub>12</sub>
<i>S</i> <sub>12</sub>	Indium Corporation	US	33,30%	96583,32	9.4	866667	$M_{11}$
<i>S</i> <sub>18</sub>	Molex	US	33,30%	96583,32	9.4	866667	$M_{11}$
<i>S</i> <sub>16</sub>	Lucas Milhaupt Global Brazing Solutions	US	33,30%	96583,32	9.4	866667	<i>M</i> <sub>11</sub>
<i>S</i> <sub>11</sub>	Hunan Jinhao Aluminum Industrial Co.	CN	33,30%	999	0.0052	8400000	<i>M</i> <sub>5</sub>
<i>S</i> <sub>22</sub>	Zhangqiu Metallic Pigment Co.	CN	33,30%	999	0.0055	7200000000	<i>M</i> <sub>5</sub>
<i>S</i> <sub>7</sub>	Chengdu Nuclear 857 New materials Co.	CN	33,30%	999	0.004	24000000000	<i>M</i> <sub>5</sub>
<i>S</i> <sub>23</sub>	Zhengzhou Dongyao Nano Materials Co.	CN	33,30%	1318,68	0.55	52000000	<i>M</i> <sub>6</sub>
<i>S</i> <sub>11</sub>	Hunan Jinhao Aluminum Industrial Co.	CN	33,30%	1318,68	0.35	12000000	<i>M</i> <sub>6</sub>
<i>S</i> <sub>17</sub>	Luoyang Tongrun Info Technology Co.	CN	33,30%	1318,68	0.34	360000000	<i>M</i> <sub>6</sub>
<i>S</i> <sub>17</sub>	Luoyang Tongrun Info Technology Co.	CN	33,30%	1678,32	0.9	12000000	<i>M</i> <sub>7</sub>
<b>S</b> <sub>7</sub>	Chengdu Nuclear 857 New materials Co.	CN	33,30%	1678,32	0.67	1200000000	$M_7$
<i>S</i> <sub>6</sub>	Chengdu Huarui Industrial Co.	CN	33,30%	1678,32	1.5	24000000	$M_7$
<i>S</i> <sub>17</sub>	Luoyang Tongrun Info Technology Co	CN	33,30%	156523,32	0.4	360000000	<i>M</i> <sub>8</sub>
<i>S</i> <sub>5</sub>	Changsha Easchem Co.	CN	33,30%	156523,32	2	12000000000	<i>M</i> <sub>8</sub>
<i>S</i> <sub>20</sub>	Shanghai Ruizheng Chemical	CN	33,30%	156523,32	5	1000000	<i>M</i> <sub>8</sub>

	Technology Co.						
<i>S</i> <sub>17</sub>	Luoyang Tongrun Info Technology Co	CN	33,30%	19980	0.017	360000000	<i>M</i> 9
<i>S</i> <sub>4</sub>	Cangzhou Lockeheed Petroleum Machinery Co.	CN	33,30%	19980	0.03	18000000	<i>M</i> <sub>9</sub>
<i>S</i> <sub>23</sub>	Zhengzhou Dongyao Nano Materials Co.	CN	33,30%	19980	0.5	52000000	<i>M</i> 9

## **Geographical profile**

According to supply profile, the supplying countries are: China (CN), Germany (GM), Japan (JP), Korea (KR), Netherland (NL) and United States (US). The supplying mass and ratio from each country were calculated from supply profile and stated in table below.

 Table 29: Materials supplying amount and ratio in corresponding to supplying countries (based on the data from "Supply profile")

Materials supplying ratio & countries	CN	GM	JP	KR	NL	US
M <sub>1</sub>	100%	0%	0%	0%	0%	0%
<i>M</i> <sub>2</sub>	0%	0%	0%	33%	50%	17%
M <sub>3</sub>	0%	0%	0%	33%	50%	17%
M <sub>4</sub>	0%	0%	0%	33%	50%	17%
<i>M</i> <sub>5</sub>	100%	0%	0%	0%	0%	0%
M <sub>6</sub>	100%	0%	0%	0%	0%	0%
<i>M</i> <sub>7</sub>	100%	0%	0%	0%	0%	0%
M <sub>8</sub>	100%	0%	0%	0%	0%	0%
Mg	100%	0%	0%	0%	0%	0%
<i>M</i> <sub>10</sub>	42%	0%	26%	31%	0%	0%
M <sub>11</sub>	0%	0%	0%	0%	0%	100%
<i>M</i> <sub>12</sub>	33%	33%	0%	0%	0%	33%

After the supplying countries being determined, data for following impact parameters were collected: diplomatic relation between each supplying country and France, bilateral economic

exchange between each supplying country and France, and stability / ease doing business score of each supplying country (Table 30). Standards for diplomatic relation are listed in methodology chapter. As the fact that France is having a comprehensive strategic partnership with China (French Ministry of foreign affairs and international development, 2013) and a strategic partnership with the United States (Juppé & Paal, 2011), I gave a mark of 0.5 to FR-CN and FR-US. From my understanding, France is having partnership relation with Japan and Korea as well. At the same time, Germany, Netherland and France are all members of the European Union. That's why I gave mark of 0 to FR-GM, and FR-NL. The bilateral economic exchange is a sum of 1) export of France to supplying country, 2) import of France to supplying country, 3) Tourist income from supplying country, 4) stock investment of France in the supplying country, 5) stock investment of the supplying country in France and 6) turnover of French companies in the country (French Gov., 2015a). In this application, the general score of stability / ease doing business is an average from following indicators: ease of doing business (The World Bank, 2016), fragile states index (FFP, 2015), estimated political stability by country (Quandl, 2015) and worldwide governance indicator (Worldbank, 2014). The data of above indicators were firstly arranged in the same order. Then they were zoomed in the same scale. Finally the average of these indicators were obtained. Details of above methods are available in previous chapters.

Table 30: Diplomatic relation, bilateral economic exchange between company located country and its supplying countries
as well as the stability general score of each supplying country

	Unit	CN	GM	JP	KR	NL	US
CL & $L_{(S_j)}$ Diplomatic relation : France &	/	0,5	0	0,5	0,5	0	0,5
CL & $L_{(S_j)}$ Bilateral economic exchange :	M€	122	239	59	19	192	410 629
France &		950	209	874	542	229	
Stability / ease doing business general score of	/	50,3	37,5	40,4	36,3	37,6	37,0
L <sub>(Sj)</sub>							

## 2.3 Criteria calculation

Criteria 3, 5, 10 of basic scenario were not calculated in this application. Criterion 3 is the substitutability which covers many technical aspects or experiments. Due to lack of time and resources, it is not calculated in this study. Criterions 5 is the legislation ban or hinder level.

As I have not found any legislation ban of selected materials in LED sector. It means all the value of this criterion is zero which means no contribution to the criticality. Hence the criterion 6 was not presented in this study. Criterion 10 is the global demand and supply ratio. Due to lack of information, this criterion is not covered in the study. The remaining criteria were presented below with one calculation example for each.

### **Criterion 1: Imbalance between demand & supply**

The imbalance between demand and supply of  $M_i$  is the ratio of  $\frac{D_{(M_i)}}{S_{(M_i)}}$ , in which the value of demand  $D_{(M_i)}$  is in Table 25 and the value of  $S_{(M_i)}$  is the sum of ASA<sub>(M\_i-S\_j)</sub> of Table 28. For example, the demand of  $M_1$  (Ce 3+: YAG) is 10 440 g (Table 25). Its supply amount  $S_{(M_1)}$  can be calculated from the data in Table 28.

$$S_{(M_1)} = \sum_{j=1}^{j=24} ASA_{(M_1 - S_j)}$$
  
=  $ASA_{(M_1 - S_{24})} + ASA_{(M_1 - S_2)} + ASA_{(M_1 - S_{15})}$   
= 12000000 g + 25000000 g + 52000000 g  
= 89000000 g

Hence, the imbalance between demand and supply of  $M_1$  is:

$$\frac{D_{(M_i)}}{S_{(M_i)}} = \frac{10\ 440\ g}{89000000\ g} = 0.000117$$

### Criterion 2: Value (functional and economic) of this material to the target product

Value is the product of functional value (FV) and economic influence (EI). Its calculation formula is as below:

$$V_{(M_i)} = FV_{(M_i)} * (EI_{(M_i)}/\$)$$

Functional value of each material  $FV_{(M_i)}$  is listed in the technical profile (Figure 27). The Economic influence can be calculated from the inputs of supply profile in Table 28 with following formula.

$$EI_{(M_i)} = \sum_{j=1}^{X} \left[ SA_{(M_i - S_j)} * Price_{(M_i - S_j)} \right]$$

For example, the average of functionality value of  $M_2$  (TMGa) is 0,2277 (technical profile Figure 27). From Table 28, we can learn that its suppliers are  $S_{19}$ ,  $S_9$  and  $S_1$ .

$$EI_{(M_2)} = \sum_{j=1}^{24} \left[ SA_{(M_2 - S_j)} * Price_{(M_2 - S_j)} \right]$$
  
=  $SA_{(M_2 - S_{19})} * Price_{(M_2 - S_{19})} + SA_{(M_2 - S_9)} * Price_{(M_2 - S_9)} + SA_{(M_2 - S_1)}$   
\*  $Price_{(M_2 - S_1)}$ 

= 249900 g \* 2
$$\left(\frac{\$}{g}\right)$$
 + 485100 g \* 2 $\left(\frac{\$}{g}\right)$  + 735000 \* 2 $\left(\frac{\$}{g}\right)$   
= 2940000 \$

The value of  $M_2$  is then

$$V_{(M_2)} = FV_{(M_2)} * \left(\frac{EI_{(M_2)}}{\$}\right)$$
  
= 0,2277 \* 2940000  
= 669438

## **Criterion 4: Environmental friendly level**

From Eco-invent, the human toxicity was obtained with a unit of kg 1,4-DCB-Eq / 1kg of material (Table 25). The environmental friendly level of one material is equal to the selected indicator multiplied by the its mass.

For example, human toxicity value of  $M_3$  (TMIn (InC3H9) is 13358,30 kg 1,4-DCB-Eq / 1kg of  $M_3$  while its demand amount is 9 960 g. Hence, its environmental friendly level is:

Environmental friendly 
$$level_{(M_3)}$$
  
=  $D_{(M_3)}$  \* selected environmental indicator  
= (9 960 g of  $M_3$ ) \*  $\frac{13358,30 \text{ kg } 1,4 - \text{DCB} - \text{Eq}}{1 \text{ kg of } M_3}$   
= 133048,68 kg of 1,4 - DCB - Eq

### **Criterion 6: Quality of relationship with suppliers**

The relationship with suppliers is marked with following five factors: quality of supplying materials, timeliness, innovation, exchange and human. With those scores, we can obtain the general relationship score between the company and its each supplier with Eq. (20) in methodology chapter. The quality of relationship is the product of general relationship score and the supplying share with Eq. (21) in methodology chapter. For example,  $M_5$  (Al) has the following suppliers:  $S_7$ ,  $S_{11}$  and  $S_{22}$ . Their supplying shares are:  $SR_{(S_7-M_5)} = 33\%$ ,  $SR_{(S_{11}-M_5)} = 33\%$ ,  $SR_{(S_{22}-M_5)} = 33\%$  (Table 28). The qualities of relationship with these suppliers (QRS) are:  $QRS_{S_7} = 0.608$ ,  $QRS_{11} = 0.256$ , and  $QRS_{S_{22}} = 0.517$ . Hence, the quality of relationship with the suppliers of  $M_5$  is:

$$QRS_{M_5} = \sum_{j=1}^{X} SR_{(S_j - M_5)}^2 \times QRS_{S_j} =$$
  
= 33.3%<sup>2</sup> × 0.608 + 33.3%<sup>2</sup> × 0.256 + 33.3%<sup>2</sup> × 0.517  
= 0.15

## **Criterion 7: Depletion of reserves**

As some of critical materials candidates contain more than one mineral, I used the related minerals' global production amount adjusted by their ratio in the candidate to represent its potential global production amount, so as its potential global reserve amount.

For example, the  $M_1$  = Ce 3+: YAG (Y<sub>3</sub>Al<sub>5</sub>O<sub>2</sub> (Ce)) contains: 18.4% of Al, 19.1% of Ce and 36.4% of Y. The global production amount of Al, Ce and Y minerals are respectively 47600 tons, 12415 tons and 7100 tons. The global reserve amount of Al, Ce, and Y minerals are respectively 62900 tons, 6454000 tons and 540000 tons. Hence the depletion of reserve of  $M_1$  is as below.

$$DoR_{M_{1}} = \frac{Global \ production \ amount \ of \ material \ (or \ related \ minerals)}{Global \ reserve \ amount \ of \ material \ (or \ related \ minerals)} = \frac{GProd_{M_{i}}}{GRsv_{M_{i}}}$$
$$= \frac{18.4\% \times 47600 \ tons + 19.1\% \times 12415 \ tons + 36.4\% \times 7100 \ tons}{18.4\% \times 62900 \ tons + 19.1\% \times 6454000 \ tons + 36.4\% \times 540000 \ tons} = 0,00952$$

# **Criterion 8: Geo-relation (political and bilateral economic exchange) between supplying and buying countries**

This criterion needs the input from supplier profile and geographic profile. For example,  $M_{10}$  (alumina / sapphire) has suppliers of  $S_8$ ,  $S_{21}$  and  $S_{14}$ . These three suppliers are respectively from  $L_{(S_8)}$  (China),  $L_{(S_{21})}$  (Korea) and  $L_{(S_{14})}$  (Japan) with supplying ratio  $SR_{(S_j-M_{10})}$  of 42%, 31% and 26% (Table 28). The supplying ratio in corresponding to supplying countries for each material is assembled in Table 29. The diplomatic score between the company located country CL (France) and the three supplying countries are all 0.5. The bilateral economic exchange amounts between the company located country (France) and the three supplying countries are all 0.5. The bilateral economic euros.

Based on the Eq.23 in methodology chapter, here is:

$$\begin{aligned} Geo - relation_{M_{10}} &= \frac{Diplomatic \ score_{M_{10}}}{Economic \ bilateral \ exchange \ (M \ €)_{M_{10}}} \\ &= \frac{\sum_{j=1}^{24} (SR_{(S_j - M_{10})} \times Diplomatic \ score_{CL - L_{(S_j)}})}{\sum_{j=1}^{24} (SR_{(S_j - M_{10})} \times Economic \ bilateral \ exchange_{CL - L_{(S_j)}})} \\ &= \frac{42\% \times 0.5 + 31\% \times 0.5 + 26\% \times 0.5}{42\% \times 122950 + 31\% \times 19542 + 26\% \times 59874} \\ &= 0,0000097 \end{aligned}$$

## **Criterion 10: Stability of supplying country**

Let us still take  $M_{10}$  as example. Its suppliers' information is stated above. The stabilities of its supplying countries China, Korea and Japan are respectively 50.3, 36.3 and 40.4 (Table 30). Hence the stability of supplying countries of  $M_{10}$  is as below.

Stability of supplying country<sub>M<sub>10</sub></sub> =  
= 
$$\sum_{j=1}^{24} (SR_{(S_j - M_{10})} \times Stability general score_{L_{(S_j)}})$$
  
= 42% × 50.3 + 31% × 36.3 + 26% × 40.4  
=43,31

If we applied the same formula to calculate the stability in the European Commission's criticality study, then the stability of supplying countries of  $M_{10}$  is as below.

Stability of supplying country<sub>M<sub>10</sub></sub> =  
= 
$$\sum_{j=1}^{24} (SR_{(S_j - M_{10})}^2 \times Stability general score_{L_{(S_j)}})$$
  
=  $42\%^2 \times 50.3 + 31\%^2 \times 36.3 + 26\%^2 \times 40.4$   
= 15.09

The reason to demonstrate the second way to calculate the stability is to show that it is possible to adapt other indicators under this methodology.

## **Criterion 11: Recycling rate**

The contribution of recycling rate to the criticality is calculated as below:

$$1 - Recycling rate_{M_i}$$

The recycling rate of each material is showed in Table 25 which is based on the recycling rate of their corresponding mineral elements. For example, the contribution of recycling rate of  $M_{11}$  is:

$$1 - Recycling rate_{M_{11}} = 1 - 43\% = 0.57$$

## 3. Results

### 3.1 Results presentation

With outputs of eight criteria demonstrated above, following data treatment was then applied. Firstly, it is to arrange all the criteria in the order of positive correlation. Then I settled 20% as the criticality threshold. It is also possible to settle the threshold otherwise. Settlement of threshold represents the subjectivity of users as well as personalization of model. We can see how results evolve if we change 20% critical to 30% or 50%. What users need to do is to modify the cell of threshold in Excel tool that proposed by this thesis and the results are changed automatically in the model. Based on the criticality threshold, the relative value of all materials in terms of each criterion is obtained. Finally, the above value is adjusted with arc tan with an interval from 0 to  $\pi$  with the purpose of better visualization and comparison of different data. The results adjusted with exponential function are available in Appendices.



Figure 30: Criticality of materials of LED general result presentation with contribution score of each criterion: 20% critical as threshold, adjusted by arc tan function

Figure 30 represents the general score of criticality as well as contribution from each criterion. From this figure, we can briefly see which criteria contributed more than others to the criticality for each material and which materials are more critical than others.

As the threshold was settled as 20% and there are 12 candidates, the top three candidates as critical materials are: TMGa, TMAl and Alumina. They are showed in the part A of Figure 31. The rest were separated into group medium (B) and group less (C) critical according to their general criticality scores. The reason to separate them into different groups is to have better presentation of results. When there are 12 or even more candidates, it is not clear to present all in the same figure. I.E. When intervals of scores are too different, it is difficult to show the small ones in the same figure. It is also more efficient for us to see which materials are in the group of most critical, medium critical and least critical and to work on a specific group. The reason to use radar chart is to better present contribution of criticality of each criterion to each material when there are more than three criteria.



Figure 31: Radar charts of criticality of materials which are divided into three groups

## 3.2 Sensitivity analysis and completeness of study

## Sensitivity analysis

The following information is considered constant in the sensitivity analysis: materials list, material ratio in the product, supplying ratio of each supplier, suppliers list, supplying ratio of each supplier and location of suppliers. After that, 12 inputs were extracted as the vector  $x = (x_1, x_2, ..., x_{12})$ , in which  $x_1$  = selected environmental indicator,  $x_2$  = recycling rate,  $x_3$  = global production amount,  $x_4$  = global reserve amount,  $x_5$  = accessible primary supply amount,  $x_6$  = planned targets (need) amount for company,  $x_7$  = function value offered by this material to the product,  $x_8$  = price of material offered by each supplier,  $x_9$  = relation score with supplier,  $x_{10}$  = stability of each supplying country,  $x_{11}$  = diplomatic relation between

supplier country and buyer country,  $x_{12}$  = economic bilateral exchange between supplying country and buying country. The outputs are represented as vector:  $y = (y_1, y_2, ..., y_9)$ .  $y_1 =$ Criterion 1: Imbalance between demand & supply,  $y_2$  = Criterion 2: Value,  $y_3$  = Criterion 4: Environment friendly level,  $y_4$  = Criterion 6: Quality of relationship with suppliers,  $y_5$  = Criterion 7: Depletion of reserves (prod/reserve),  $y_6$  = Criterion 8: Geo relation (politic+economic),  $y_7$  = Criterion 10: Stability of supplying country,  $y_8$  = Criterion 11: Recycling rate of related raw materials,  $y_9$  = General score of criticality.

Firstly, I increased 10% and 100% of each input for all material at the same time. The increases of 10% and 100% of  $x_1$ ,  $x_3$ ,  $x_6$ ,  $x_7$ ,  $x_8$ ,  $x_{10}$ ,  $x_{11}$  separately lead to an increase of 10% and 100% of corresponding outputs:  $y_3$ ,  $y_5$ ,  $(y_1, y_2, y_3)$ ,  $y_2$ ,  $y_2$ ,  $y_7$  and  $y_6$ . The increases of 10% and 100% of  $x_4$  lead to an change of -9% and -92% correspondingly of its output  $y_5$ . The increases of 10% and 100% of  $x_5$  and  $x_{12}$  lead to changes of -9% and -50%of corresponding output  $y_1$  and  $y_6$ . As the general score of criticality  $(y_9)$  is a relative value, an increase of above inputs do not affect it at all. Except for above regular input-output relations, the outputs of  $x_2(y_8)$  and  $x_9(y_4)$  are irregular. When I increased 10% of  $x_2, y_8$ changes from -11% to 0 and  $x_9$  changes from -3.8% to 0.8%. When I increased 100% of  $x_2$ ,  $y_8$  changes from -113% to 0 and  $x_9$  changes from -33.6% to 8.6\%. That is because certain inputs (recycling) of  $x_2$  are zero which makes its increases null as well. When I increased 10% of  $x_9$ , its output  $y_4$  increased 10% regularly. However when I increase 100% of  $x_9$ , its output  $y_4$  increased from 57% to 99% and  $x_9$  changes from -3.1% to 11.8%. That is because increase of 100% has exceeded the threshold of certain  $x_9$  values. To conclude, this sensitivity analysis confirmed the preconception about relativity of the proposed methodology. If we change the same proportion of non-zero inputs of all the materials at the same time and if the change does not surpass their intervals, the general score of criticality of materials remain the same.

Secondly, I increased 10% and 100% of one input for only one material. It is also closer to real situation where one or more impact parameters like price, demand amount, etc. of certain materials vary. However, when I change the inputs  $x_6$  of one material, mass ratios of other materials are changed as well. So does for  $x_7$  because the sum of  $x_7$  or  $x_6$  of all materials is supposed to be 1. When I change stability of supplying countries  $x_{10}$  of one material, the

stability score of other materials which have the same supplying countries will change as well. So does  $x_9$ . When the increases surpass the interval of inputs  $(x_2, x_7, x_9, x_{10}, x_{11})$ , I used the maximum or minimum value to replace the 100% increase amount. For example, if one supplier's general relation score is 0.634, its 100% increased amount is 1.268 which surpassed 1. Then, I used 1 as the increased input to calculate the sensibility. Here are two sensibility analysis examples of  $M_1$  and  $M_4$  (results are in Figure 32).



Figure 32: Examples of sensibility analysis for two materials. Part a: changes of general score of the criticality of M1 when each input increased 10% or 100% individually. Part b: changes of general score of the criticality of M2 when each input increased 10% or 100% individually. Part c: changes of criticality ranking of M1 when each input increased 10% or 100% individually. Part c: changes of M2 when each input increased 10% or 100% individually.

According to the figure, following conclusions can be drawn. 1) Different inputs are impacting differently to the general score of criticality. For example, x12, x11, x10, x9 and x2 are impacting more than other inputs on both M1 and M2 in this scenario. Incensement of x2, x4, x5 and x12 decreased the criticality while the others increased. In another word, increasing x2, x4, x5, x12 or decreasing x1, x3, x6, x7, x8, x9, x10, x11allow to decrease the criticality of one material which is also coherent to the diagnosis part. 2) The same input may have different impacts on different materials. For example, 100% increase of x4 is influencing the criticality dropped two places while same change did not impact the ranking of M4 at all. One word to be added is that, the above relations are under the situation where all criteria have the same importance.

## Completeness

There are 39 impact parameters in total offered by the methodology (Figure 8) where 22 were selected for basic scenario. The LED application covered 77% of the impact parameters listed in the basic scenario. The impact parameters related to legislation ban were not covered in LED application was because no corresponding threaten was discovered in a predictable period. As they did not contribute to criticality in this scenario, it is not interesting to show them in the radar charts. The ones related to global demand and supply ratios were not covered due to lack of data. The ones related to substitutability were not covered due to lack of expert opinions and time; meanwhile, the substitutability is important to criticality.
# **CHAPTER 7**

# **DISCUSSIONS AND PERSPECTIVES**

### Simplicity & Comprehensiveness

Simplifying the metrics reduces the precision of results, although it decreases the amount of required data which makes the studies easier to be conducted. Some authors (Poulizac, 2013) mentioned that metrics used in current assessments are often static. Even some may include a dynamic aspect; it is still not enough to reflect the complexity and interactions of the market. Most assess tools require a lot of data and professional knowledge, which increases the difficulty and uncertainty to execute them. It seems like a paradox: when the metrics or tools do not include enough indicators, they may not be comprehensive enough. In addition, most metrics need professional opinions from experts or the opinions of decision-makers which are subjective. Different experts may offer different information which would lead to different results. Compared to a static system, the consideration of dynamic aspect affords better support for forecast studies (Candelise et al., 2011b). Therefore one limitation of the current static methods is that dynamic changes are not considered (Knoeri et al., 2013), e.g. feedback or reaction from actors facing critical material problems was not taken account (Poulizac, 2013). Another limitation is that economic approaches aim for long term, which is not the industrial priority. Both dynamic involvement and long term consideration can make criticality study more comprehensive, however that also means more time and resources to complete the work.

### Order of criticality research

The ultimate goal of conducting the criticality study is to find solutions or mitigation approaches to the actual or potential critical materials issues. The factors which can provoke or influence the criticality of materials should be thoroughly studied, not only for the purpose of criticality determination model but also for finding mitigation approaches. At present, the pre-phase before criticality methodology development is lacking (the thesis aims at filling up this gap). Without this diagnostic phase of criticality, there is no way to judge if the definition of criticality is representative or not. The criticality assessment methodology cannot be verified. Furthermore, each mitigation approach is connected to the impact parameters of the criticality. An overall diagnostic of the parameters which may influence the criticality can provide ideas for finding solutions. It also becomes a guideline to check if all aspects have been considered or not.

# Potential use of Material Flow Analysis (MFA) in criticality study

Material Flow Analysis (MFA) can be used as a tool to support useful information in the post critical materials studies and also afford data for the methodology (Figure 26). For instance, in the methodology developed by Öko-Institut (2009), pre-consumer recycling and post-consumer recycling were two major fields of the "recycling" parameter. MFA can offer the detailed value of pre-consumer or post-consumer flow.

#### Obstacles or difficulties for conducting criticality studies

When we carry out a critical material study, the following obstacles / issues need to be taken into account. Firstly, with the complexity of product design and supply chain, it is more and more difficult to know the exact materials contained in the current product, not mentioning upstream information about sourcing and extraction. The various sub-contractors and confidentiality have made or make the supply chain more and more complex. It makes the evaluation methodology less accurate and the data more difficult to obtain. Secondly, a comprehensive critical material study requires financial or human resources. For example, the studies of the European Commission and the Department of Energy are supported by government. They both have experts from various fields to help them. Thirdly, data is always a big obstacle. Lack of data or low quality of data make the study more difficult. Some authors (Department of Energy, 2011a) stated that there are big gaps or uncertainties between the actual reserves, resources, production or consumption data of China and the reality. In addition, lag of data updating also decreases the credibility of the study. When the supply of certain materials is concentrated in one country, the policies in that country might also have big influence on that material's market. Then interferences of the government in the market might become an obstacle or even raise the critical risk, like the palladium crisis of Russia. Over interference from the government can reduce market transparency and even confuse the information. Without correct information, it is more difficult to detect or mitigate the criticality related issues. Fourthly, the interactions of all the activities of different interested parties make the situation changing and dynamic. Among the potential changes caused by criticality, some are the solutions or mitigation approaches taken by different organizations which will probably concern technical, political and other aspects. The 20th century Cobalt

crisis which occurred in Zaire was a good example to show how the material's criticality can influence the global supply chain, production technologies, national policies and even one country's stability (Alonso et al., 2007). The criticality phenomenon can also stimulate the reopening of new or existed mining sites. At global level, the consuming countries or the supply chain stakeholders might have to consider how their own resources would change the global supply chain. Mineral prospection technologies may also be improved thanks to these facts. All those dynamic reactions are difficult to model.

#### **Indicators and calculation method**

Certain indicators and calculations stated in the quantitative evaluation model were proposed by the author. Due to knowledge and personal limitations, they may not be the best or maybe inaccurate. Better indicators may be developed in the future. Hence I would like to say that the indicators, calculation methods or even the methodology proposed in this thesis may not be the best for evaluating criticality, but only remain one available option for other researchers and industries.

## Weightings & Subjectivity

In applying the evaluation model, determining weightings and building scenarios without subjectivity is difficult. In terms of model development, a space (specific cells in the Excel tool) can be left to adjust the weighting. It is challenging to provide weightings during calculation for certain criteria. The final result presentation is a radar chart containing 11 criteria in the basic scenario. Different weightings of criteria might change completely the final result. In the methodology, there are two places where weighting is needed: functionality and four aspects of substitutability. We can use the Delphi Method (Brown, 1968) to provide weighting in which marks are given by a group of distinguished experts in limited rounds anonymously. Analytic Hierarchy Process (AHP) (Bhushan & Rai, 2004) or the mixture of these two methods is also an option for weighting.

## **Threshold setting**

Two places were needed to give thresholds: substitutability evaluation and criteria normalization. The thresholds in the substitutability evaluation are related to the requirements of products from clients and other corresponding sectors. It can be obtained from the product's technical specifications or technical experts in industries. The threshold of criterion

for the final results presentation is the extreme value of each criterion before arriving at the critical area. Two ways were proposed to determine the thresholds for criteria. The first way is to use a certain ratio such as 20:80 or 30:70. It means we consider a certain ratio of values surpassing the critical threshold. The second way is to settle each threshold by experts. This is similar to the Delphi method. A problem such as "how much should we settle the threshold of this criterion?" can be given to a panel of experts. After a determined number of rounds, we can use the median value in the final round as the threshold.

### Potential use of proposed methodology

It is possible to apply the framework of the methodology for adaptation at general sector level by modifying the scope of the study and certain impact parameters. For example, we can replace the demand of a product of a company by the global demand for this product. The suppliers will be replaced by the general suppliers in the world or for a country. The relation to the suppliers will be difficult to quantify and can be replaced by geo-relation with the supplying countries. The stability of the supplying countries can be calculated using the indicator such as "Ease of doing business" or "Stability" with those countries' supplying shares. Some other criteria's calculations might need to be adjusted as well.

Another potential use of this methodology is to determine the criticality of components instead of one raw material. As showed in the LED application, certain materials contain more than one metal and the criticality of these materials can also be determined. The ways used in LED application to treat these materials can be used for components as well.

#### Limitations and points to be improved

There are still many limitations of above two applications and things remained to be improved. In terms of limitations, how the decision of industries can be influenced by the results of criticality is not studied. The second application is based on a hypothetical company whose situation is based on the Philips lighting. The LED materials and demand data are based on a DOE report of Endurant LED lamp as well as the assumption of their market share. None of the data are first hand. Three suppliers were selected randomly from Internet for each material while it may be different with real case in terms of numbers and suppliers. Hence, the results of criticality of LED materials cannot be used directly by others, neither the ones of permanent magnet applications. As author is not expert of LED, I might make

mistakes or leave out some points while making LED materials and technical profiles. However, the above limitations will not become a problem if a real company wants to apply this methodology. The panel of experts who have joined the survey contains only four members. However, by considering that the objective is searching expertise instead of statistics, it was acceptable. While I built the diplomatic table, the results were not reviewed by related experts. Data delay is also a problem. Sometimes it is impossible to get the current data. For example, some annual reports from the USGS or the World Bank are released the year after. At the end, the methodology is supposed to be suitable for non-metals as well; however, non-metal materials were not tested in above applications.

About the three research gaps stated previously, this thesis was focused on two first gaps. Works on evaluation models of other scenarios and links among different phases should be established later. For the methodology, only one example of evaluation model was illustrated in detail. Others remain to be developed. About gap 3 - links among different phases (Figure 3), I only came up brief thoughts of how to establish those links, but detail works have not been conducted yet. In details, finding the appropriate weightings of criteria can increase a lot the accuracy of criticality score. In both applications, all the criteria were assumed equally important to general criticality score which means they have the same weighting in the results data treatment. It may be not appropriate in some real situations. Whether to find one weighting system of criteria for all cases in general or to determine the weightings case by case independently still remains discussible. What I proposed in the model is to leave a place where people can modify the weightings values. Another thing to be improved is affording recommendations for mitigation measures. They are not yet integrated automatically in the evaluation model. For now, the mitigation measures can be added manually by checking all the measures collected from reviewed studies. Those are also prospective future works. Calculations of the model have not been justified yet. It remains possible that researchers change or improve certain indicators in the future. In addition, as only the calculation of the developed model is arranged under Excel for now, however, it will be better to achieve the automation of whole methodology or model in the future. At the end, feedbacks after industries applying the criticality evaluation model can be used to improve the methodology or model. How other stakeholders, such as governments or other sectors, should cooperate based on results of criticality studies can be future work as well.

# **CHAPTER 8**

# CONCLUTION

#### **Research questions and answers**

This thesis was guided by following research questions:

- **What have been done in the criticality research area**?
- 4 Q1: How to define criticality of materials?
- **Q2**: How to determine the criticality of materials (at product level)?

Regarding pre-research question, this research question led to a scoping review and was answered mainly in chapter 2. This answer severed as baselines for following research works. To summary, the term critical firstly appeared in an ex-classified official memorandum called "critical imported commodities" in 1974. Then 34 years later, the National Research Council developed a criticality matrix to evaluate the criticality of materials which was then used as basic concept by the European Commission (Europe) and the Department of Energy (United States) in their critical materials studies in 2010. In the same year, a rare earth issue was triggered by China's export policy which might be one of the motivations of above two critical materials studies. At the same time, the term critical was separated from other similar terms such as strategic, important, precious, scare and so on and drew more and more attention. On the other hand, if we use the term critical to match material issues happened in the history, we can tell that the phenomenon of criticality was not novel; however, its research activities just started and remain new.

Until now, majority of studies focused on determining which materials are critical for an area / administrative region, certain technologies or material family. Several criticality evaluation methodologies were also developed for above different scopes. Some follow-up works on solutions or countermeasures were also conducted. However, a pre-phase about criticality diagnosis (which parameters make materials critical or analysis of criticality terms) was barely worked on. Evaluation of criticality of materials at product level was missing. The connections among diagnosis, evaluation methodology and solutions were not established.

Besides, above statements were based on reviewed studies which did not contain documents written in languages that I do not speak, confidential or industrial ones that I do not have access to or even those omitted during review process. The statements, including answers to other questions, were limited by my education background as well as time scheduled for review.

Regarding research question 1, the definition proposed by this thesis is: *criticality of a material is a relative value of the interaction among the importance of the material to the object, the imbalance between demand and accessible supply of the actor, and accessibility of the material. Criticality is reinforced with abrupt changes or situations where actors are not able to adapt.* 

All the materials are important in a certain degree. The word "relative" showed that I do not ignore the importance of other materials. It is to highlight the ones which need urgent or more attentions under certain conditions, which are called critical. The word "object" contains following information: To whom the criticality of materials is analyzed: a product, a group of materials, a technology, a company, a country or others. The object can also be interpreted as scope or context of criticality. It projects the dynamic concept (personalization of definition) and highlights that criticality results can be totally different in different situations. "Actors" means the organization behind the target object. The last sentence "reinforced with abrupt changes or situations where actors are not able to adapt" contains following information: 1) no materials can be critical forever; 2) less time that the actors possess to respond to issues caused by criticality means higher criticality when other variables remain the same; 3) criticality is also influenced by adaptability of the actor to issues caused by criticality or new situations. i.e. If the actor has already been prepared for possible situations and has capacity to respond to them, the criticality will no longer be the same. Except for above complementary information, "importance, the imbalance between demand and supply, and accessibility" are three dimensions influencing the criticality directly.

The comprehensive case study of rare earth responded to above definition.

Regarding research question 2, a Materials Criticality Profiling Methodology (MCPM) for general case and a quantitative evaluation model for basic scenario were developed for determining the criticality of materials at product level.

The methodology offers guidelines or frameworks to carry on a critical material study:

- Decide the target product. This is a first scope limitation. When a product is decided, corresponding materials and functionalities required are decided as well. The specific product corresponds to the word "object" of the definition.
- Decide the material candidate pool. This is a second scope limitation. We can choose to analyze a part of materials which appeared more critical based on experience, opinions of experts or other filtrations. We can also choose to analyze all the corresponding materials if it is possible.
- Build the scenario. Scenario here contains two meanings. The first meaning relates to selection of impact parameters. The methodology contains a criticality impact parameters pool. We can select the ones appeared more appropriate under specific circumstance and the ones that we are able to evaluate. The second meaning of scenario relates to assemble all the information like preferences or interests, such as a forecast, a possible case, a case with environmental or financial preferences, etc. and describe it.
- Build calculation model. Based on impact parameters selected in the scenario and stated preferences, we then develop criteria to evaluate the criticality.
- Select indicator for certain parameters. More than one method can be available to evaluate certain criteria sometime and it leads to a selection of appropriate indicators.
- Input data in calculation model. With above steps, the required data is determined. We then collect the data and input them in the calculation model.
- Analyze results. Obtain the general score of criticality, how criticality is contributed and what countermeasures should be taken based on integrated results of calculation model.

The quantitative evaluation model for basic scenario is a proposition and a demonstration of above methodology. The basic case means no preference on any aspect and focus on current situation. The impact parameters selected in basic scenario are those more often caused material crisis recently and possible to evaluate. Based on this scenario, a calculation model was build. It contains following eleven criteria: imbalance between demand and supply, value, substitutability of the material to the product, environmental friendly level, legislation ban or hinder level, quality of relationship with suppliers, depletion of reserves, geo-relation, global

demand to supply ratio, stability of supplying country and recycling rate. Data treatment for results presentation includes following steps: put outputs of criteria calculation in right order; take relative value of each criterion; make them all positive and within same baseline. Results were finally presented in a general score (or histogram diagram), radar charts and descriptive measures. Sensitivity and completeness analysis were also proposed.

Two applications, permanent magnet and LED, demonstrated how the model works and confirmed the feasibility. They also served to improve the evaluation model.

## List of contributions of this thesis

It is the first time to bring the criticality at product level. There are two main contributions: 1) a new definition of criticality including a comprehensive diagnosis of criticality and 2) a new evaluation methodology at product level. In detail, they contain the list below:

- An overall map of criticality research is established. It shows what has been done and what needs to be done in this domain.
- A comprehensive diagnosis of criticality (a phase before criticality evaluation methodology development) was established at the first time. The mechanism and parameters which influence the criticality were presented.
- A new definition of criticality of materials at product level is developed at the first time.
- A new evaluation methodology of criticality of materials at product level is proposed at the first time.
- A quantitative criticality evaluation model for basic scenario (a complementary of above methodology) was developed.
- Methods for various criteria calculation were proposed, as well as data treatment.
- A new way to approach the dynamic in the criticality evaluation is presented.

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# Supporting information for review chapter

N.	Reference with issued year	Institution	Region of institution	Type of institution	Geographic scope	Phase
1	(National Research Council, 2008)	National Research Council	U.S.	Other research/ consultation institutions	US	mid
2	(European commission, 2010)	European commission	U.S.	Governmental	EU	mid
3	(Statistics Netherlands, 2010)	Statistics Netherlands	Netherlands	Governmental	Dutch	post
4	(DOE, 2010)	DOE	U.S.	Governmental	US	mid
5	(DOE, 2011)	DOE	U.S.	Governmental	US	mid
6	(Resnick Institute, 2011)	Resnick Institute Report	U.S.	Collegiate	US - general	post
7	(APS & MRS, 2011)	APS&MRS	U.S.	Inter-institutions	Global	mid
8	(Silberglitt, 2013)	National defense research institute / RAND	U.S.	Governmental	US	post
9	(OUSDATL, 2013)	Office of the undersecretary of defense for acquisition, technology and logistics/ Department of defense	U.S.	Governmental	US	mid
10	(APS & MRS, 2011)	MIT, APS, MRS	U.S.	Inter-institutions	US	mid
11	(Hatch, 2011)	Individual (Technology metals research)	U.S.	Other research/ consultation institutions	Global	post
12	(Massari, 2013)	University	Italy	Collegiate	Global	post
13	(Speirs, 2012)	ERC	UK	Collegiate	UK-General	/
14	(Speirs, 2011)	ERC	UK	Collegiate	UK	/
15	(Speirs, 2013a)	ERC	UK	Collegiate	UK	/

Table S 1: Table S1: Information of primary review scope (48 studies) - Part a

16	(Speirs, 2013B)	ERC	UK	Collegiate	UK	mid
17	(Candelise, 2011)	University	UK	Collegiate	UK	/
18	(DEFRA, 2012)	DEFRA	UK	Governmental	UK	post
19	(Smith, 2012)	WRAP	UK	Governmental	UK	post
20	(Rademaker, 2013	University	Netherlands	Collegiate	Global	post
21	(Barreau, 2013)	Commissariat général à la stratégie et à la prospective	France	Governmental	France	post
22	(Moss, 2011)	Öko-Institut e.V	Germany	Other research/ consultation institutions	Global	post
23	(Nuss, 2014)	Yale University	U.S.	Collegiate	Global and U.S.	mid
24	(Graedel, 2012)	Yale university	U.S.	Collegiate	Corporate, national, global	mid
25	(Nassar, 2011)	Yale university	U.S.	Collegiate	Corporate, national, global	mid
26	(Baché, 2013)	VTT	FINLAND	Governmental	EU	post
27	(European Commission, 2014)	EC	EU	Governmental	EU	mid
28	(Parthemore, 2011)	Center for a New American Security (CNAS)	U.S.	Other research/ consultation institutions	US	mid
29	(Thomason, 2010)	IDA	U.S.	Other research/ consultation institutions	US	mid
30	(Goe, 2014)	Rochester Institute of Technology	U.S.	Collegiate	US	mid
31	(Morley, 2008)	Resource Efficiency Knowledge transfer network	UK	Other research/ consultation institutions	UK	post
32	(Poulizac, 2013)	MIT	U.S.	Collegiate	Global	mid
33	(S.L.C, 2011)	S.L.C	U.S.	Governmental	US	/

			IIK			
34	(Moss, 2011	EC JRC-IET	Australia	Collegiate	EU	mid
35	(Roelich, 2014)	University of Leeds	UK	Collegiate	Global	mid
36	(Cleveland, 1993)	Center for Energy and Environmental Studies and Department of Geography	U.S.	Collegiate	U.S.	/
37	(Erdmann, 2011)	Institute for Futures studies and technology assessment (IZT) and Yale university	Germany, U.S.	Collegiate	Global	mid
38	(The White House, 1974)	The White House	U.S.	Governmental	U.S.	/
39	(Kooroshy, 2010)	HCSS (Hague for Strategic Studies)	Netherlands	Other research/ consultation institutions	Global	/
40	(Congressional Budget Office, 1983)	CBO (congressional budget office)	U.S.	Governmental	U.S.	/
41	(GPO, 1979)	The White House	U.S.	Governmental	U.S.	/
42	(Commission of the European Communities, 2008)	EC	EU	Governmental	EU	post
43	(Knoeri, 2013)	University of Leeds, EMPA, Karlsruhe Institute of Technology, Helmholtz-Institute Ulm for Electrochemical Energy Storage	UK, Switzerland, Germany	Collegiate	/	mid
44	(Duclos, 2010)	GE	U.S.	Company(GE)	GE	mid
45	(IW Consult, 2009)	IW Consult	Germany	Other research/ consultation institutions	Germany	mid
46	(NEDO, 2009)	NEDO (Shinko research)	Japan	Other research/ consultation institutions	Japan	mid
47	(RWI/ISI/BGR, 2007)	RWI/ISI/BGR study	Germany	Inter-institutions	Germany	mid
48	(Angerer, 2009)	IZT & Fraunhofer	Germany	Other research/ consultation institutions	Germany	/

N.	Reference with issued year	Research scope	Highlighted sector
1	(National Research Council, 2008)	US economy	US economy
2	(European commission, 2010)	determine critical raw materials for EU	economy
3	(Statistics Netherlands, 2010)	dependency if the Dutch economy on 44 critical materials	Dutch economy
4	(DOE, 2010)	examines the role of RE metals and other materials in the clean energy economy	general clean energy technologies
5	(DOE, 2011)	11) roles of REE and others in Clean energy technology	
6	(Resnick Institute, 2011)	Sustainable energy	solar/photovoltaic, permanent magnets
7	(APS & MRS, 2011)	Energy / emerging technologies	energy / emerging technologies
8	(Silberglitt, 2013)	concerns of production, concerns of reliability of supply raised by governance issues	manufacturing
9	(OUSDATL, 2013)	stockpile requirement	defense sector and essential civil sector
10	(APS & MRS, 2011)	new energy technologies	new energy technologies
11	(Hatch, 2011)	rare earths supply, demand	Rare earths
12	(Massari, 2013)	international market, rare earth	RE market and strategies
13	(Speirs, 2012)	availability, low-carbon economy	general low carbon energy technologies

# Table S 2 : Information of primary review scope (48 studies) - Part b

14	(Speirs, 2011) availability, low-carbon economy general thin film PV		general thin film PV	
15	(Speirs, 2013a)	material availability, low carbon economy	omy electric vehicles (batteries, motors), wind turbines	
16	(Speirs, 2013B)	availability, comparison of material criticality studies - methodologies and results	/	
17	(Candelise, 2011)	availability	general thin film PV	
18	(DEFRA, 2012)	national resource strategy	strategic Energy Technology (SET) Plan, Clean technologies	
19	(Smith, 2012)	recovery, EU CM	WEEE	
20	(Rademaker, 2013	Solution of criticality	permanent magnet	
21	(Barreau, 2013)	supply issues	transport, energy	
22	(Moss, 2011)	Future sustainable technologies:	EEE Technologies Photovoltaic Technologies Battery Technologies Catalysts	
23	(Nuss, 2014)	basic metals, 2008	iron related industry	
24	(Graedel, 2012)	criticality Methodology	/	
25	(Nassar, 2011)	copper family	copper family	
26	(Baché, 2013)	supply chain analysis	ICT and electronics sectors	
27	(European Commision, 2014)	raw materials	economy	
28	(Parthemore, 2011)	mitigating risk of US dependence on CM	economy	
29	(Thomason, 2010)	stockpile requirement	defense	
30	(Goe, 2014)	identify CM	photovoltaics	
31	(Morley, 2008)	resource availability	economy	

32	(Poulizac, 2013)	criticality assessment and mitigation	mining economics	
33	(S.L.C, 2011)	promote domestic production	domestic sectors in US	
34	(Moss, 2011	assess shortage risk	low-carbon energy technologies	
35	(Roelich, 2014)	dynamic material criticality assessment	low-carbon electricity	
36	(Cleveland, 1993)	scarcity	/	
37	(Erdmann, 2011)	review of major approaches and analyses	/	
38	(The White House, 1974)	political guild lines	Imported commodities	
39	(Kooroshy, 2010)	Scarcity	/	
40	(Congressional Budget Office, 1983)	vulnerability	defense and industrial	
41	(GPO, 1979)	political guidelines	/	
42	(Commission of the European Communities, 2008)	response (political approaches) to criticality	/	
43	(Knoeri, 2013)	dynamic assessment model development	/	
44	(Duclos, 2010)	identify CM (materials at risk of supply constraints or price increases) for GE	industrial (company)	
45	(IW Consult, 2009)	vulnerabilities and risks of material supply	economy	
46	(NEDO, 2009)	analyze rare metal supply; identify projects for substitution	economy	
47	(RWI/ISI/BGR, 2007)	ram materials supply; long term supply and demand	Economy	
48	(Angerer, 2009)	foresee potential demand surges, help to ease pressure on the raw materials markets	general emerging technologies	

N.	Reference with issued year	Material type	Developed criticality assessment methodology :Yes(Y) or Not(N)	Recommendatio n of mitigation approaches : Yes(Y) or Not(N)	Designation a list of critical materials : Yes(Y) or Not(N)
1	(National Research Council, 2008)	Nonfuel mineral, mineral product and alloys	Y (criticality matrix)	Y	Y
2	(European commission, 2010)	raw materials	Y	Y	Y
3	(Statistics Netherlands, 2010)		Ν	Y (for further research)	N (EC14+3 extra covered)
4	(DOE, 2010)	metals	Y	Y	Y
5	(DOE, 2011)	REE and other metals	N (same as 2010)	Y (similar with 2010)	Y
6	(Resnick Institute, 2011)		Ν	Υ	N (selected 18 materials)
7	(APS & MRS, 2011)	chemical elements with novel use	Ν	Y	Ν
8	(Silberglitt, 2013)	CE materials	/	/	Y (EC41, other lists "important raw materials")
9	(OUSDATL, 2013)	non-fuel materials	Y (shortfall computing methodology)	Y	Y (shortfall list)
10	(APS & MRS, 2011)	Cases studies of RE, Cadmium/Telluriu m, Helium	N	Y	N (but case study of RE, cadmium/ tellurium, helium)
11	(Hatch, 2011)	RE	Ν	/	N (study of RE)
12	(Massari, 2013)	RE	Ν	/	N ( study of RE)

# Table S 3 : Information of primary review scope (48 studies) - Part c

13	(Speirs, 2012)	metals	N	N	N (study of Co, Ga, Ge, In, Li, PGM, REE, Se, Ag, Te)
14	(Speirs, 2011)	indium, tellurium			Ν
15	(Speirs, 2013a)	Li, Neodymium	N (compare supply to demand for availability)	Ν	Ν
16	(Speirs, 2013B)		/	/	Ν
17	(Candelise, 2011)	indium, tellurium	Ν	/	Ν
18	(DEFRA, 2012)	ram materials (EU CM)	Ν	Y	Ν
19	(Smith, 2012)	ram materials	Ν	Y (for market failure)	N(use EC14)
20	(Rademaker, 2013	REE	Ν	Y (recycling)	Ν
21	(Barreau, 2013)	metals	N (but with own criteria)	Y (with solutions)	Ν
22	(Moss, 2011)	metals	Y(classification and prioritization)	Y	N (but selected 11 critical materials)
23	(Nuss, 2014)	Iron and its principal alloying elements	Ν	Ν	N (study of V, Cr, Mn, Fe, Nb)
24	(Graedel, 2012)	Metal	Y	Ν	Ν
25	(Nassar, 2011)	Copper family	N (applied)	Ν	Ν
26	(Baché, 2013)	raw materials	N ( but supply chain analysis methodology)		N ( EC14)
27	(European Commision, 2014)	(abiotic + biotic) raw materials	Ν	Y	Y
28	(Parthemore, 2011)	minerals	Ν	Υ	N (study of REE, Nb, Ta, Re, Ga, Li)
29	(Thomason, 2010)	minerals	Υ	/	Y (but shortage)
30	(Goe, 2014)	metals	Υ	Y	Y (designated, no cover list)

31	(Morley, 2008)	metals	Y (material security)	Y	Y
32	(Poulizac, 2013)	/	Y (M5:(Materials mining market model)	Y	Ν
33	(S.L.C, 2011)	/	Ν	Y	Ν
34	(Moss, 2011	metals	N (bottleneck risk)	Y	Y
35	(Roelich, 2014)	/	Y	/	Ν
36	(Cleveland, 1993)	natural resource	N (but scarcity indicators)	/	Ν
37	(Erdmann, 2011)	non-fuel materials	Ν	Ν	Ν
38	(The White House, 1974)	Imported commodities	Ν	Y	Ν
39	(Kooroshy, 2010)	mineral	Ν	Ν	N (but studied 15 materials)
40	(Congressional Budget Office, 1983)	minerals	N (but vulnerability determination illusion)	Y	N (but analyzed 8 materials)
41	(GPO, 1979)	/	/	/	Y (not available)
42	(Commission of the European Communities, 2008)	/	Ν	Y	Ν
43	(Knoeri, 2013)	raw materials	Y (conceptual framework)	/	Ν
44	(Duclos, 2010)	resources	Y	/	Y (not available)
45	(IW Consult, 2009)	raw materials	Y	/	Y (not available)
46	(NEDO, 2009)	rare metals	Y	/	Y (not available)
47	(RWI/ISI/BGR, 2007)	raw materials	Y	/	Y (not available)
48	(Angerer, 2009)	mineral raw materials	Y (vulnerability)	/	N (but important material list)

# Supporting information for chapter 6 Part II LED Application

## A. Data collection

#### a. Materials profile to produce one LED

The materials components of a LED are based on the DOE report (Scholand & Dillon, 2012). The production of 1kg of diodes generates 0.37 kg of waste where of 0.04 kg are calculated to be unused raw materials. So it means that the production loss of raw material is 4% (eco-invent). However, the dataset used by Eco-invent has been adjusted. It has an input of 1.04 kg of raw material for 1 kg of diode. The LED in this study is a white light LED. The substrates where grown the GaN can be sapphire, silicon carbide (SiC), bulk GaN, silicon, germanium, borosilicate glass, poly-cristal aluminium nitride (AIN), zinc oxide and diamand (Scholand & Dillon, 2012). Among them, sapphire substrate makes up 80% of LED substrates (Compound Semiconductor, 2011).

To manufacture a wafer of Three-Inch Sapphire, it requires 16.6 g of alumina (Al2O3) (equivalent to aluminium oxide in Ecoinvent) and 830.0 g of diamond slurry ) (equivalent to zeolite, slurry in Ecoinvent) (Scholand & Dillon, 2012).



Figure S 1 : main mass flow to produce 3-intch wafer (based on the source: (Scholand & Dillon, 2012))

One of the three ways (see figure) to generate white light for LED is to add a Ce<sup>3+</sup> : YAG phosphor. It is because the combination between the yellow light from Ce<sup>3+</sup> : YAG and the blue light from semi-conductor turns to white light (CCT > 4000K, CRI ~70 – 80) through the eyes of human (Setlur, 2009). One LED needs 0.192 mm<sup>3</sup> of this phosphor (Scholand & Dillon, 2012). With a density of 4.55 g/cm<sup>3</sup>(Saint-Gobain, 2014), one pcLED requires 0.0008736 grams.

$$m = \rho * v = 4.55 \frac{g}{cm^3} * 0.192 \ mm^3 = 4.55 \frac{g}{cm^3} * (0.192 * 10^{-3}) \ cm^3 = 0.0008736 \ g$$

Table S 4 : metal elements contained materials'	consumption for making one LED	(calculation based
on DOE(Scholand & Dillon, 20	012) report and above information)	

Com	ponent	Material	Consumptio	Unit	eqv Ecoinvent material
			n amount		-
LE D	Quantum well &	TMGa (Ga(CH3)3)	0,12250	g/LE D	gallium, semiconductor- grade, at plant
	n-p layers	TMIn (InC3H9)	0,00083	g/LE D	indium, at regional storage
		TMAl (C6H18Al2)	0,00025	g/LE D	aluminum, production mix, at plant
	Metal contact	Al	0,00025	g/LE D	aluminum, production mix, at plant
		Ni	0,00033	g/LE D	nickel, 99.5%, at plant
		Ag	0,00042	g/LE D	silver, from combined gold- silver production, at refinery
		Ti	0,03917	g/LE D	titanium dioxide, production mix, at plant
		W	0,00500	g/LE D	palladium, secondary, at precious metal refinery
	Sapphire substrate	Alumina	1,38333	g/LE D	aluminum oxide, at plant
	Solder layer	AuSn solder	0,02417	g/LE D	gold, from combined metal production, at refinery
	Submount	Alumina	0,01350	g/LE D	aluminum oxide, at plant
	Phosphor	Ce 3+: YAG (Y3Al5O12(Ce ))	0,00087	g/LE D	
	Wire bond	Gold	0,00006	g/LE D	gold, from combined metal production, at refinery
Total pcLE	materials consur D	nption for one	1,59068	g/LE D	

Metal elements		LED			]	LED package	:	Consumption	Mass
consumption								amount	percentage
&								g/ LED	
Components									
Metal element	Quantum well	Metal contact	Sapphire	Solder	Phosphor	Submount	Wire bond		
name	&		Substrate	layer					
	p-n layers								
Ag		0,00042						0,00042	0,0471%
Al	0,00009	0,00025	0,73178		0,00016	0,00714		0,73943	83,6215%
Au				0,01506			0,00006	0,01512	1,7097%
Ce					0,00017			0,00017	0,0188%
Ga	0,07460							0,07460	8,4368%
In	0,00060							0,00060	0,0674%
Ni		0,00033						0,00033	0,0377%
Sn				0,00911				0,00911	1,0305%
Ti		0,03917						0,03917	4,4293%
W		0,00500						0,00500	0,5654%
Y					0,00032			0,00032	0,0358%
Tot	al metal element	s consumptions	(without con	ncerns of pro	duction) for a	one LED		0,88425	100,0000%

Table S 5 : metal elements' consumptions to produce ach component of one LED: based on the DOE report (Scholand & Dillon, 2012)

	Ag	AI	Au	Ce	Ga	In	Ni	Sn	Ti	w	Y
Ce 3+: YAG (Y3Al5O12(Ce))		18,4%		19,1%							36,4%
TMGa (Ga(CH3)3)					60,9%						
TMIn (InC3H9)						71,9%					
TMAl (C6H18Al2)		37,5%									
Al		100,0%									
Ni							100,0%				
Ag	100,0%										
Ti									100,0%		
W										100,0%	
Alumina		52,9%									
AuSn solder			62,3%					37,7%			
Gold			100,0%								

Table S 6 : The percentage of each mineral element contained in each material to be analyzed

Material element code		unit	ME_1	ME_2	ME_3	ME_4	ME_5	ME_6	ME_7	ME_8	ME_9	ME_10	ME_11
Materials element	nt	/	Ag	Al	Au	Ce	Ga	In	Ni	Sn	Ti	w	Y
Mass ratio of ma in the product	aterial	%	0,04710%	83,62150%	1,70970%	0,01880%	8,43680%	0,06740%	0,03770%	1,03050%	4,42930%	0,56540%	0,03580%
Material amoun needed to be pur for 1 LED	t chase	ър	0,00042	0,73943	0,01512	0,00017	0,0746	0,0006	0,00033	0,00911	0,03917	0,005	0,00032
Human toxicity (Eco- invent)	HT	kg 1,4- DCB- Eq /1kg of material	310940	162,78	1093,3	395,35	1773,6	18579	2992,9	348,33	0,21438	2305,9	4,3496
Exo-toxicity (Eco-invent)	ET	kg 2,4- D-Eq/ /1kg of material	8 107,700000	3,7724	440290	395,35	27,512	1697,6	151,82	205,69	0,76478	89,699	15,523
GWP 100a (Eco-invent)	GWP	kg CO2- Eq//1kg of material	441,52	8,3723	9139,4	11,251	203,46	154,28	10,897	17,174	4,5484	446,84	55,497
Environmental selected	HT	kg 1,4- DCB- Eq /1kg of material	310940	162,78	1093,3	395,35	1773,6	18579	2992,9	348,33	0,21438	2305,9	4,3496
<b>Recycling rate</b>		%	47%	46%	32%	0%	0%	0%	41%	60%	24%	53%	0%
Global reserve amount		tons	520000	62900	55000	6454000	1000000	11000	81000000	4800000	1120300	3300000	540000
Global production amount	on	tons	26000	47600	2800	12415	273	199	2630000	294000	209000	81400	7100
Global stock am	ount	tons	na	na	na	na	na	na	na	na	na	na	na
Global demand		tons	na	na	na	na	na	na	na	na	na	na	na

 Table S 7 : Materials elements information (HT, ET, GWP data are from Eco invent 2.2; Recycling rate, Global reserve amount and Global production amount

 data are from USGS, except for: Recycling rate of Ce, Indium and Y (Buchert et al., 2012), recycling

## b. Technical profile

Survey

Standards:

- aij = 1, General functionality "i" is as same important as the General functionality "j" to LED
- aij = 3, General functionality "i" is slightly importanter than the General functionality "j" to LED
- aij = 5, General functionality "i" is more important than the General functionality "j" to LED
- aij = 7, General functionality "i" is much more important than the General functionality "j" to LED
- aij = 9, General functionality "i" is extrem more important than the General functionality "j" to LED

Survey from Expert 1 (Gunhee):

		j = 1	j = 2	j = 3	j = 4	j = 5	j = 6	j = 7
		GF1	GF2	GF3	GF4	GF5	GF6	GF7
i = 1	GF1	1	1	1	1	3	5	5
i = 2	GF2	1	1	1	1	3	3	5
i = 3	GF3	1	1	1	3	3	3	5
i = 4	GF4	1	1	0,333	1	1	1	1
i = 5	GF5	0,333	0,333	0,333	1	1	1	1
i = 6	GF6	0,2	0,333	0,333	1	1	1	1
i = 7	GF7	0,2	0,2	0,2	1	1	1	1

Table S 8 : Matrix 1: Importance of General functionality to LED - AHP methods according to expert 1

Table S 9 : Matrix 2: Importance of functionality to its super hierarchy - GF3 according to expert 1

		j = 1	j = 2
		F3	F4
i = 1	F3	1	1
i = 2	F4	1	1

Table S 10 : Matrix 3: Importance of functionality to its super hierarchy - GF4 according to expert 1

		j = 1	j = 2	j = 3	j = 4
		F5	F6	F7	F8
i = 1	F5	1	1	1	1
i = 2	F6	1	1	1	3
i = 3	F7	1	1	1	1
i = 4	F8	1	0,333	1	1

Table S 11 : Matrix 4: Importance of functionality to its super hierarchy - GF5 according to expert 1

		j = 1	j = 2	j = 3
		F9	F10	F11
i = 1	F9	1	1	1
i = 2	F10	1	1	1
i = 3	F11	1	1	1

Table S 12 : Matrix 5: Importance of functionality to its super hierarchy - GF6 according to expert 1

		j = 1	j = 2	j = 3	
		F12	F13	F14	
i = 1	F12	1	1	1	
i = 2	F13	1	1	1	
i = 3	F14	1	1	1	

						Contrib	ution of	each mate	erial to ea	ach functi	onality			
			Phosphor	QWS	P-N Junc	tions		Me	etal conta	cts		Substrate	Solder	Wire
			M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8	M_9	M_10	M_11	M_12
	Functionality	Sum	Ce 3+:											
		should -	YAG	TMGa		TMAI								
		1	(Y3Al5O	(Ga(CH3	TMIn	(C6H18A							AuSn	
		-	12(Ce))	)3)	(InC3H9)	12)	Al	Ni	Ag	Ti	W	Alumina	solder	Gold
F1	Have energy gaps to emit the photons for blue light	100%	0%	20%	20%	20%	5%	5%	3%	3%	0%	15%	3%	6%
F2	Have energy gaps to transmit the photons	100%	0%	25%	25%	20%	0%	0%	0%	0%	0%	15%	0%	15%
F3	Have the matching lattice structure (atomic level)	100%	0%	25%	25%	25%	0%	0%	0%	0%	0%	25%	0%	0%
F4	Have enough binding between atoms to make layers binded (atomic level)	100%	0%	30%	30%	30%	0%	0%	0%	0%	0%	10%	0%	0%
F5	Connect different surfaces (metal contact & solder, solder&wire ) firmly	100%	0%	10%	10%	10%	0%	0%	0%	0%	0%	30%	20%	20%
F6	Have low electrons escape in the connecting surfaces (metal contact & solder, solder&wire)	100%	0%	30%	30%	30%	0%	0%	0%	0%	0%	10%	0%	0%
F7	Not be melted during usage (solder)	100%	0%	10%	10%	10%	0%	0%	0%	0%	0%	70%	0%	0%
F8	Have (solder) strong enough as connector	100%	0%	0%	0%	0%	15%	15%	15%	15%	15%	0%	10%	15%
F9	Be hard enough to support the other devices (submount, substrate)	100%	0%	20%	20%	20%	0%	0%	0%	0%	0%	30%	0%	10%
F10	Dissipate heat efficiently enough to maintain the right temperature of above devices (submount, substrate)	100%	0%	10%	10%	10%	10%	10%	10%	10%	10%	0%	10%	10%
F11	No leakage of electricity (submount, substrate)	100%	0%	0%	0%	0%	5%	5%	5%	5%	5%	30%	25%	20%
F12	Appear yellow light in order to generate the white light after mixing with the blue light emitted by quantum wells	100%	40%	25%	25%	10%	0%	0%	0%	0%	0%	0%	0%	0%
F13	Have the emission peak in the required range (while appearing yellow light)	100%	0%	30%	40%	30%	0%	0%	0%	0%	0%	0%	0%	0%
F14	Have the excitation range (while appearing yellow) light which covers the wavelenght of the light emitted by quantum wells	100%	0%	30%	40%	30%	0%	0%	0%	0%	0%	0%	0%	0%
F15	Conduct the electrons as efficiently as possible to alimente the quntum wells (wire, metal contacts, solder)	100%	0%	30%	40%	30%	0%	0%	0%	0%	0%	0%	0%	0%

Table S 13 : Contribution of each material to each functionality according to expert 1

Survey from Expert 2 (Heesoo):

		j = 1	j = 2	j = 3	j = 4	j = 5	j = 6	j = 7	
		GF1	GF2	GF3	GF4	GF5	GF6	GF7	_
i = 1	GF1	1	1	1	1	3	3	5	
i = 2	GF2	1	1	1	1	1	3	3	
i = 3	GF3	1	1	1	1	1	3	5	
i = 4	GF4	1	1	1	1	1	1	3	
i = 5	GF5	0,333	1	1	1	1	1	1	
i = 6	GF6	0,333	0,333	0,333	1	1	1	1	
i = 7	GF7	0,2	0,333	0,2	0,333	1	1	1	

Table S 14 : Table S14: Matrix 1: Importance of General functionality to LED - AHP methods according to expert 2

Table S 15 : Matrix 2: Importance of functionality to its super hierarchy - GF3 according to expert 2

		j = 1	j = 2
		F3	F4
i = 1	F3	1	1
i = 2	F4	1	1

Table S 16 : Matrix 3: Importance of functionality to its super hierarchy - GF4 according to expert 2

		j = 1	j = 2	j = 3	j = 4
		F5	F6	F7	F8
i = 1	F5	1	1	1	1
i = 2	F6	1	1	1	1
i = 3	F7	1	1	1	1
i = 4	F8	1	1	1	1

Table S 17 : Matrix 4: Importance of functionality to its super hierarchy - GF5 according to expert 2

		j = 1	j = 2	j = 3
		F9	F10	F11
i = 1	F9	1	1	1
i = 2	F10	1	1	1
i = 3	F11	1	1	1

		j = 1	j = 2	j = 3
		F12	F13	F14
i = 1	F12	1	1	1
i = 2	F13	1	1	1
i = 3	F14	1	1	1

Table S 18 : Matrix 5: Importance of functionality to its super hierarchy - GF6 according to expert 2

						Contrib	ution of	each mate	erial to ea	ach functi	onality			
			Phospho	QWS	P-N Junc	tions		Me	etal conta	cts		Substrate	Solder	Wire
			M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8	M_9	M_10	M_11	M_12
	Functionality	Sum	Ce 3+:											
		should -	YAG	TMGa		TMAI								
		1	(Y3Al5O	(Ga(CH3	TMIn	(C6H18A							AuSn	
		1	12(Ce))	)3)	(InC3H9)	12)	Al	Ni	Ag	Ti	W	Alumina	solder	Gold
F1	Have energy gaps to emit the photons for blue light	100%	0%	20%	20%	20%	5%	5%	5%	5%	5%	15%	0%	0%
F2	Have energy gaps to transmit the photons	100%	0%	35%	25%	20%	0%	0%	0%	0%	0%	10%	0%	10%
F3	Have the matching lattice structure (atomic level)	100%	0%	25%	25%	25%	0%	0%	0%	0%	0%	25%	0%	0%
F4	Have enough binding between atoms to make layers binded (atomic level)	100%	0%	30%	30%	20%	0%	0%	0%	0%	0%	20%	0%	0%
F5	Connect different surfaces (metal contact & solder, solder&wire ) firmly	100%	0%	5%	5%	5%	0%	0%	0%	0%	0%	30%	25%	30%
F6	Have low electrons escape in the connecting surfaces (metal contact & solder, solder&wire )	100%	10%	20%	20%	30%	0%	0%	0%	0%	0%	10%	10%	0%
F7	Not be melted during usage (solder)	100%	0%	10%	10%	10%	0%	0%	0%	0%	0%	50%	20%	0%
F8	Have (solder) strong enough as connector	100%	0%	0%	0%	0%	10%	10%	10%	10%	10%	0%	35%	15%
F9	Be hard enough to support the other devices (submount, substrate)	100%	0%	15%	20%	15%	0%	0%	0%	0%	0%	30%	0%	20%
F10	Dissipate heat efficiently enough to maintain the right temperature of above devices (submount, substrate)	100%	0%	10%	10%	5%	15%	15%	15%	15%	15%	0%	0%	0%
F11	No leakage of electricity (submount, substrate)	100%	0%	0%	0%	0%	0%	10%	0%	10%	5%	30%	25%	20%
F12	Appear yellow light in order to generate the white light after mixing with the blue light emitted by quantum wells	100%	60%	10%	20%	10%	0%	0%	0%	0%	0%	0%	0%	0%
F13	Have the emission peak in the required range (while appearing yellow light)	100%	0%	30%	40%	30%	0%	0%	0%	0%	0%	0%	0%	0%
F14	Have the excitation range (while appearing yellow) light which covers the wavelenght of the light emitted by quantum wells	100%	0%	30%	40%	30%	0%	0%	0%	0%	0%	0%	0%	0%
F15	Conduct the electrons as efficiently as possible to alimente the quntum wells (wire, metal contacts, solder)	100%	0%	40%	30%	30%	0%	0%	0%	0%	0%	0%	0%	0%

# Table S 19 : Contribution of each material to each functionality according to expert 2

Survey from Expert 3 (Kyunghyun):

		j = 1	j = 2	j = 3	j = 4	j = 5	j = 6	j = 7
		GF1	GF2	GF3	GF4	GF5	GF6	GF7
i = 1	GF1	1	1	1	1	1	3	5
i = 2	GF2	1	1	1	3	3	5	5
i = 3	GF3	1	1	1	1	1	5	5
i = 4	GF4	1	0,333	1	1	1	1	1
i = 5	GF5	1	0,333	1	1	1	1	1
i = 6	GF6	0,333	0,2	0,2	1	1	1	1
i = 7	GF7	0,2	0,2	0,2	1	1	1	1

Table S 20 : Matrix 1: Importance of General functionality to LED - AHP methods according to expert 3

Table S 21 : Matrix 2: Importance of functionality to its super hierarchy - GF3 according to expert 3

		j = 1	j = 2
		F3	F4
i = 1	F3	1	1
i = 2	F4	1	1

Table S 22: Matrix 3: Importance of functionality to its super hierarchy - GF4 according to expert 3

		j = 1	j = 2	j = 3	j = 4
		F5	F6	F7	F8
i = 1	F5	1	1	1	1
i = 2	F6	1	1	1	1
i = 3	F7	1	1	1	1
i = 4	F8	1	1	1	1

		j = 1	j = 2	j = 3
		F9	F10	F11
i = 1	F9	1	1	1
i = 2	F10	1	1	1
i = 3	F11	1	1	1

Table S 23 : Matrix 4: Importance of functionality to its super hierarchy - GF5 according to expert 3

Table S 24 :: Matrix 5: Importance of functionality to its super hierarchy - GF6 according to expert 3

		j = 1	j = 2	j = 3											
		F12	F13	F14											
i = 1	F12	1	1	1											
i = 2	F13	1	1	1											
i = 3	F14	1	1	1											
						Contrib	ution of	each mate	erial to ea	ach functi	onality				
-----	--	----------	---------	---------	----------	---------	----------	-----------	-------------	------------	---------	-----------	--------	------	--
			Phospho	QWS	P-N Junc	tions		Me	tal conta	cts		Substrate	Solder	Wire	
			M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8	M_9	M_10	M_11	M_12	
	Functionality	Sum	Ce 3+:												
		should =	YAG	TMGa		TMAI									
		1	(Y3AI5O	(Ga(CH3	TMIn	(C6H18A							AuSn		
			12(Ce))	)3)	(InC3H9)	12)	Al	Ni	Ag	Ti	W	Alumina	solder	Gold	
F1	Have energy gaps to emit the photons for blue light	100%	0%	20%	20%	20%	5%	5%	2%	2%	1%	15%	5%	5%	
F2	Have energy gaps to transmit the photons	100%	0%	30%	30%	20%	0%	0%	0%	0%	0%	10%	0%	10%	
F3	Have the matching lattice structure (atomic level)	100%	0%	30%	30%	30%	0%	0%	0%	0%	0%	10%	0%	0%	
F4	Have enough binding between atoms to make layers binded (atomic level)	100%	0%	35%	35%	20%	0%	0%	0%	0%	0%	10%	0%	0%	
F5	Connect different surfaces (metal contact & solder, solder&wire ) firmly	100%	0%	5%	5%	5%	0%	0%	0%	0%	0%	30%	25%	30%	
F6	Have low electrons escape in the connecting surfaces (metal contact & solder, solder&wire)	100%	0%	20%	20%	20%	0%	0%	0%	0%	0%	20%	20%	0%	
F7	Not be melted during usage (solder)	100%	0%	10%	10%	10%	0%	0%	0%	0%	0%	50%	10%	10%	
F8	Have (solder) strong enough as connector	100%	0%	0%	0%	0%	15%	20%	15%	20%	20%	0%	5%	5%	
F9	Be hard enough to support the other devices (submount, substrate)	100%	0%	20%	20%	20%	0%	0%	0%	0%	0%	20%	10%	10%	
F10	Dissipate heat efficiently enough to maintain the right temperature of above devices (submount, substrate)	100%	0%	5%	5%	5%	5%	20%	15%	10%	10%	5%	10%	10%	
F11	No leakage of electricity (submount, substrate)	100%	0%	0%	0%	0%	10%	10%	10%	5%	5%	20%	20%	20%	
F12	Appear yellow light in order to generate the white light after mixing with the blue light emitted by quantum wells	100%	55%	20%	15%	10%	0%	0%	0%	0%	0%	0%	0%	0%	
F13	Have the emission peak in the required range (while appearing yellow light)	100%	0%	35%	35%	30%	0%	0%	0%	0%	0%	0%	0%	0%	
F14	Have the excitation range (while appearing yellow) light which covers the wavelenght of the light emitted by quantum wells	100%	0%	35%	35%	30%	0%	0%	0%	0%	0%	0%	0%	0%	
F15	Conduct the electrons as efficiently as possible to alimente the quntum wells (wire, metal contacts, solder)	100%	0%	35%	35%	30%	0%	0%	0%	0%	0%	0%	0%	0%	

# Table S 25 :: Contribution of each material to each functionality according to expert 3

## Survey from Expert 4 (Hyun): Primary test

	j = 1	j = 2	j = 3	j = 4	j = 5	j = 6	j = 7
	GF1	GF2	GF3	GF4	GF5	GF6	GF7
i = 1 GF1	1	1	1	2	5	5	5
i = 2 GF2	1	1	2	3	3	3	3
i = 3 GF3	1	0,5	1	1	1	1	1
i = 4 GF4	0,5	0,333	1	1	1	1	1
i = 5 GF5	0,2	0,333	1	1	1	1	1
i = 6 GF6	0,2	0,333	1	1	1	1	1
i = 7 GF7	0,2	0,333	1	1	1	1	1

Table S 26 :: Matrix 1: Importance of General functionality to LED - AHP methods according to expert 4

Table S 27 : Matrix 2: Importance of functionality to its super hierarchy - GF3 according to expert 4

		j = 1	j = 2
		F3	F4
i = 1	F3	1	1
i = 2	F4	1	1

Table S 28 : Matrix 3: Importance of functionality to its super hierarchy - GF4 according to expert 4

		j = 1	j = 2	j = 3	j = 4
		F5	F6	F7	F8
i = 1	F5	1	1	1	1
i = 2	F6	1	1	2	2
i = 3	F7	1	0,5	1	1
i = 4	F8	1	0,5	1	1

Table S 29 : Matrix 4: Importance of functionality to its super hierarchy - GF5 according to expert 4

		j = 1	j = 2	j = 3
		F9	F10	F11
i = 1	F9	1	1	1
i = 2	F10	1	1	1
i = 3	F11	1	1	1

Table S 30 : Matrix 5: Importance of functionality to its super hierarchy - GF6 according to expert 4

		j = 1	j = 2	j = 3
		F12	F13	F14
i = 1	F12	1	1	1
i = 2	F13	1	1	1
i = 3	F14	1	1	1

						Co	ntribution	of each mat	erial to each	functional	ity			
			Phosphor	QW	S P-N Junct	ions			Metal contac	t		Substrate	Solder	Wire
			M_1	M_2	M_3	M_4	M_5	M_6	M_7	M_8	M_9	M_10	M_11	M_12
	Functionality	Sum should	Ce 3+: YAG											
		- 1	(Y3Al5O12(	TMGa	TMIn	TMAI							AuSn	
		- 1	Ce))	(Ga(CH3)3)	(InC3H9)	(C6H18Al2)	Al	Ni	Ag	Ti	W	Alumina	solder	Gold
F1	Have energy gaps to emit the photons for blue light	100%	0%	20%	20%	20%	2%	5%	5%	5%	1%	10%	5%	7%
F2	Have energy gaps to transmit the photons	100%	0%	25%	25%	25%	0%	0%	0%	0%	0%	10%	10%	5%
F3	Have the matching lattice structure (atomic level)	100%	0%	30%	20%	20%	0%	0%	0%	0%	0%	30%	0%	0%
F4	Have enough binding between atoms to make layers binded (atomic level)	100%	0%	30%	30%	30%	0%	0%	0%	0%	0%	10%	0%	0%
F5	Connect different surfaces firmly	100%	0%	20%	10%	10%	0%	0%	0%	0%	0%	30%	15%	15%
F6	Have low electrons escape in the connecting surfaces	100%	0%	30%	30%	30%	0%	0%	0%	0%	0%	10%	0%	0%
F7	Not be melted during usage	100%	0%	20%	20%	20%	0%	0%	0%	0%	0%	40%	0%	0%
F8	Have tensile connection (solder) of different parts	100%	0%	0%	0%	0%	10%	10%	10%	10%	10%	0%	20%	30%
F9	Be hard enough to support the other devices	100%	0%	15%	15%	15%	0%	0%	0%	0%	0%	50%	0%	5%
F10	Dissipate heat efficiently enough to maintain the right temperature of above devices	100%	0%	10%	10%	10%	10%	10%	10%	10%	10%	0%	10%	10%
F11	Be insulated for the purpose of safety and avoid the electrons running off	100%	10%	0%	0%	0%	5%	5%	5%	5%	5%	30%	15%	20%
F12	Appear yellow light in order to generate the white light after mixing with the blue light emitted by quantum wells	100%	70%	10%	10%	10%	0%	0%	0%	0%	0%	0%	0%	0%
F13	Have the emission peak in the required range	100%	0%	30%	35%	35%	0%	0%	0%	0%	0%	0%	0%	0%
F14	Have the excitation range which covers the wavelenght of the light emitted by quantum wells	100%	0%	30%	35%	35%	0%	0%	0%	0%	0%	0%	0%	0%
F15	Conduct the electrons as efficiently as possible to alimente the guntum wells	100%	0%	30%	35%	35%	0%	0%	0%	0%	0%	0%	0%	0%

# Table S 31 : Contribution of each material to each functionality according to expert 4

Survey results assemblage

AHP weighting calculation with tool Matlab - Calculation example

#### Matrix 1 of expert Hyun

This matrix is for evaluating the weighting of general functionalities to LED. From this matrix, we know that:

n = 7RI = 1.32

From Matlab, we obtain that

$$\lambda \max(A) = 7.2801$$
$$CI = 0.0467$$
$$CI$$

$$CR = \left(\frac{OI}{RI}\right) = 0.0354$$

*Vector of*  $\lambda = (0.6619, 0.5723, 0.2772, 0.2186, 0.1913, 0.1913, 0.1913)$ 

So the weight of GFs to LED is as below:

Weight (	0,2873	0,2484	0,1203	0,0949	0,0830	0,0830	0,0830	)
GF to LED	GF1	GF2	GF3	GF4	GF5	GF6	GF7	

There into, the weight of GF1 to LED is obtained as formula:

$$\frac{0.6619}{0.6619 + 0.5723 + 0.2772 + 0.2186 + 0.1913 + 0.1913 + 0.1913} = 0.2873$$
$$\sum_{L=1}^{L=7} W_{(GF_L)} = 1$$

Because the consistency index CR = 0.0354 < 0.1, Hyun's subjective evaluation of the importance of general functionality to LED is consistent.

#### Matrix 2 of expert Hyun

This matrix is for evaluating the weights of F3 and F4 to GE3. From this matrix, we know that:

n = 2

$$RI = 0$$

From Matlab, we obtain that

$$\lambda \max(A) = 2$$
$$CI = 0$$

*Vector of* 
$$\lambda = (0.7071, 0.7071)$$

So the weight of GFs to LED is as below:

Weight (	0.5000	0.5000	)
F to GF3	F3	F4	

Thereinto, the weight of F3 to GF3 is obtained as formula:

$$\frac{0.7071}{0.7071 + 0.7071} = 0.5000$$

Under GF3, there are F3 and F4, the l is from 3 to 4.

$$\sum_{l=3}^{l=4} W_{(F_l)} = 1$$

Because there are two dimensions in this matrix, the subjective is always considered Consistent.

As we know that

$$W_{(GF_3)} = 0.1203$$

So the

Weight (	0.0602	0.0602	)
F to LED	F3	F4	

Weightings of other functionalities to LED were obtained in the same method. After treating other matrix with the same method, the weightings are assembled as below:

	Kyunghyun	Heesoo	Gunhee	Hyun	Average
GF1	0,1850	0,2227	0,2287	0,2873	0,2309
GF2	0,2613	0,1748	0,2096	0,2484	0,2235
GF3	0,2029	0,1913	0,2407	0,1203	0,1888
GF4	0,1098	0,1524	0,1143	0,0949	0,1179
GF5	0,1098	0,1156	0,0743	0,0830	0,0957
GF6	0,0672	0,0823	0,0702	0,0830	0,0757
GF7	0,0640	0,0608	0,0623	0,0830	0,0675

Table S 32 : Weighting of General Functionalities to the LED (The maximum Consistency ratio is 0.03which is less than 0.1. Thus the consistency of these weighting is acceptable)

Table S 33 : Weighting of functionalities to the LED (The maximum Consistency ratio is 0.02 which isless than 0.1. Thus the consistency of these weighting is acceptable)

	Kyunghyun	Heesoo	Gunhee	Hyun	Average
F1	0,185	0,2227	0,2287	0,2873	0,2309
F2	0,2613	0,1478	0,2096	0,2484	0,2168
F3	0,1015	0,0957	0,1204	0,0602	0,0945
F4	0,1015	0,0957	0,1204	0,0602	0,0945
F5	0,0275	0,0381	0,0275	0,0234	0,0291
F6	0,0275	0,0381	0,0378	0,0329	0,0341
F7	0,0275	0,0381	0,0275	0,0193	0,0281
F8	0,0275	0,0381	0,0214	0,0193	0,0266
F9	0,0366	0,0385	0,0248	0,0277	0,0319
F10	0,0366	0,0385	0,0248	0,0277	0,0319
F11	0,0366	0,0385	0,0248	0,0277	0,0319
F12	0,0224	0,0274	0,0234	0,0277	0,0252
F13	0,0224	0,0274	0,0234	0,0277	0,0252
F14	0,0224	0,0274	0,0234	0,0277	0,0252
F15	0,0640	0,0608	0,0623	0,0830	0,0675

Materials	Ce 3+: YAG	TMGa	TMIn	TMAI	AI	Ni	Ag	Ti	W	Alumina	AuSn solder	Gold	
FV	0,0123	0,2427	0,2416	0,1937	0,0189	0,0257	0,0170	0,0147	0,0128	0,1182	0,0404	0,0624	Kyunghyun
	0,0203	0,2154	0,2047	0,1794	0,0207	0,0246	0,0207	0,0246	0,0226	0,1486	0,0439	0,0473	Heesoo
	0,0094	0,2272	0,2381	0,2132	0,0184	0,0184	0,0138	0,0138	0,0069	0,154	0,0232	0,0638	Gunhee
	0,0222	0,2253	0,2239	0,2239	0,0118	0,0205	0,0205	0,0205	0,009	0,1178	0,0535	0,0515	Hyun
	0,0161	0,2277	0,2271	0,2025	0,0174	0,0223	0,0180	0,0184	0,0128	0,1346	0,0402	0,0562	Average

Table S 34 : Functionality Value (FV) of the materials to LED

#### c. Supply profile

We selected randomly three suppliers for each material. As there are some suppliers offering more than one material, the total numbers of suppliers is 24 in this study which means

X = 24

The suppliers,  $S_j$ , j = 1 to 24, are listed as below:

$$S_1 = AkzoNobel$$

 $S_2 = Beijing Yuji Science and Technology Co.$ 

- $S_3 = California Fine Wire$
- $S_4 = Cangzhou Lockedeed etroleum Machinery Co.$
- $S_5 = Changsha Easchem Co.$
- $S_6 = Chengdu Huarui Industrial Co.$
- $S_7 = Chengdu Nuclear 857 New material CO.$
- $S_8 = Crystal Applied$
- $S_9 = DOW Electronic Material$
- $S_{10} = Haraeus$
- $S_{11} =$  Hunan Jinhao Aluminium Industrial Co.
- $S_{12} = Indium corporation$
- $S_{13} = Jiangsu Plaza Premium Electric Instrument$
- $S_{14} = Kyocera$

 $S_{15} = Longkou Unity Premium Electric Instrument$ 

 $S_{16} = Lucas Milhaupt Global Brazing Solutions$ 

 $S_{17} = Luoyang Tongrun Info Technology Co.$ 

 $S_{18} = Molex$ 

 $S_{19} = SAFC Hitech$ 

 $S_{20} =$  Shanghai Ruizheng Chemical Technology Co.

 $S_{21} = STA$ 

 $S_{22} = Zhangqiu Metallic Pigment Co.$ 

 $S_{23} = Zhengzhou Dongyao Nano Material Co.$ 

 $S_{24} = Zhuhai Hanbo Trading$ 

From the Table 6, we can get the information of global production capacity of sapphire substrate in 2013. To fabricate one wafer, it requires 16.6 g of alumina. From the production capacity, we can see the alumina supplying capacity behind these suppliers.

From LED inside website, we got the market share of leader suppliers of sapphire substrates.

Table S 35 : Table S35: Market share of main suppliers of sapphire substrate based on the productioncapacity in 2013 (Lin, 2014)

Location <sup>1</sup>	Amount / M PCS	Eqv in Alumina/g	Market share
тw	1.6	26559936	19%
KR	1.2	19919952	14%
TW	1.1	18259956	13%
JP	1	16599960	12%
JP	0.9	14939964	11%
тw	0.8	13279968	9%
CN	0.7	11619972	8%
KR	0.6	9959976	7%
KR	0.6	9959976	7%
	Location <sup>1</sup> TW KR TW JP JP TW CN KR KR	Location <sup>1</sup> Amount / M PCS           TW         1.6           KR         1.2           TW         1.1           JP         1           JP         0.9           TW         0.8           CN         0.7           KR         0.6	Location <sup>1</sup> Amount / M PCS         Eqv in Alumina/g           TW         1.6         26559936           KR         1.2         19919952           TW         1.1         18259956           JP         1         16599960           JP         0.9         14939964           TW         0.8         13279968           CN         0.7         11619972           KR         0.6         9959976

<sup>&</sup>lt;sup>1</sup> The location is based on the headquarter location. It might not represent the real geographical locations of the manufacturing plants.

We randomly picked the "Crystal Apllied", "STA", and "Kyocera" as the suppliers of alumina (sapphire substrate). We assumed that the supplying ratio is based on their market share above which lead 42% from Crystal Applied, 26% from the Kyocera and 31% from STA.

According to the DOE report(Bardsley et al., 2014), the main suppliers of metal reagents (such as TMGa, TMIn, TMAI) are SAFC Hitech, Dow Electronic Material in North America, and AkzoNobel in Europe. From the annual company report of SAFC(2012), its total sales in 2012 was \$ 2 623 million with 24% share of commercial business unit. Its commercial unit's sale was around \$ 629 million. According to DOW's(2015) annual report, its Consumer Solutions' sale in 2014 was \$ 4 637 millions in which around 25% was electronic materials. Its electronic materials' sale was around \$ 1 185 million. According to AkzoNobel's (2015) 2014 annual report, 28% of the total sales were for consumer goods which include the electronic materials. That was around € 1 568 million (US \$ 1788 million).

The money exchange in this document is as below:

$$1 \in = 1.14 \text{ U.S. }$$
  
1 yuan = 0.154 US \$

We assume that their market shares of metal reagents are proportional to those listed above.

Suppliers - Revenue	Location <sup>6</sup>	Unit	Amount	Market share
SAFC	US	\$/M	629	17%
DOW	KR	\$/M	1185	33%
AkzoNobel	NL	\$/M	1788	50%

Table S 36 : Market share of main suppliers of metal reagents

We picked the three above companies as suppliers for TMGa, TMIn and TMAI. The supplying ratio is 17% for SAFC, 33% for DOW, and 50% for AkzoNobel. AKZONobel(De Kok, 2016) is offering the following prices: 2.0 \$/g for TMGa, 20 \$/g for TMI and 8\$/g for TMAI. Their TMGa production capacity is more than 20 000 kg/year. Their TMIn production capacity is more than 1000 kg/year. Their TMAI production capacity is more than 5000 kg/year.

As the fact that 1) there are so many suppliers of yellow phosphors, gold wires, metal contacts and solders; 2) we didn't find the main suppliers list with their market share; we picked up three suppliers for each material from internet.

Table S 37 : Fine gold wire suppliers

Suppliers - Revenue	Location <sup>6</sup>	Annual Supplying capacity	Market share	Supplying price (\$/g)
Jiangsu Plaza Premium Electric Instrument	CN	12 Million meters (Plaza premium, 2016)	NA	NA
Callifornia Fine Wire	US	NA	NA	NA
Haraeus	GM	NA	NA	NA

Gold for one LED is 0.00006g.

Gold density is  $19.3g/\text{cm}^3$ . The minimum diameter available from the Plaza is 0.02mm. So one meter of this gold wire is  $m = \rho * v = 19.3 \frac{g}{cm^3} * (3.14 * 0.001^2 * 100)cm^3 = 0.006g$ . It means that 12 million meter is equal to 72000g of gold.

In terms of AuSn solder, it contains usually 80% of gold and 20% of tin(Zschech, Whelan, EUROMAT, & Federation of European Materials Societies, 2005). The price of tin is 16.98 \$/kg (LME, 2016) and the price of gold is 39 719 \$/kg(Gold Price, 2016). The Hangzhou Dongzheng Industrial Company (2016) is offering a price of Tin solder wire between 2 to 8 \$/kg with a supply ability of 5 tons per week. The average of tin solder wire is then 5 \$/kg according to this supplier. If we only consider the cost of raw materials, then the AuSn solder is costing 9.4 \$/g.

$$5\left(\frac{\$}{kg}\right) \times \frac{16.98 \times 20\% + 39719 \times 80\%}{16.98} = 9357\left(\frac{\$}{kg}\right) \approx 9.4 \left(\frac{\$}{g}\right)$$

The Guangzhou Newsky Electronic Co.(2016) has a supply ability of 5000 pieces per week for its product "high quality BK 100g lead free solder" which weights 100g a and contains 30 pieces. If we ignore the accessibility of gold and use the equipment to produce AuSn solder. Then its supply ability of AuSn solder can be:

$$5000 \left(\frac{pieces}{week}\right) \times 52 \left(\frac{week}{year}\right) \times \frac{100g}{30} = 866\ 667\ \left(\frac{g}{year}\right)$$

Supplier	Locatio n <sup>6</sup>	Supplyin g ratio	Supplying amount (g)	Supplyin g price (\$/g)	Supplying capacity (g)	Material
Sj	$L_{(S_j)}$	$SR_{(S_j-M_i)}$	$SA_{(S_j-M_i)}$	Price <sub>(Mi-S</sub>	$ASA_{(M_i-S_j)}$	M <sub>i</sub>
Crystal Apllied	TW	42%	7040023,2	0.6	26559936	Sapphire substrate
STA	KR	31%	5196207,6	0.6	19919952	Sapphire substrate
Куосега	JP	26%	4358109,6	0.6 <sup>2</sup>	16599960	Sapphire substrate
SAFC	US	17%	249900	2	6800000 <sup>3</sup>	Trimethylgallium
DOW	KR	33%	485100	2	13200000	Trimethylgallium
AkzoNobel	NL	50%	735000	2	20000000	Trimethylgallium
SAFC	US	17%	1693,2	20	340000 <sup>4</sup>	Trimethylindium
DOW	KR	33%	3286,8	20	660000	Trimethylindium
AkzoNobel	NL	50%	4980	20	1000000	Trimethylindium
SAFC	US	17%	510	8	1700000 <sup>5</sup>	Trimethylalumini um
DOW	KR	33%	990	8	3300000	Trimethylalumini um
AkzoNobel	NL	50%	1500	8	5000000	Trimethylalumini um
Zhuhai Hanbo Trading	CN	33,30%	3476,52	1.25 <sup>6</sup>	12000000 <sup>7</sup>	Yellow phosphor

Table S 38 : Assemblage of suppliers' information with data source

<sup>2</sup> We assume that California Fine Wire and Haraeus have the same supplying ability of Plaza's.

11. The price of one wafer of sapphire substrate if from 10 to 100\$(Changchun Worldhawk Optoelectronics, 2016). We assume that the company get the minimum price 10\$/wafer with the big amount of purchase. One wafer requires 16.6 g of alumina, so the price is 0.6\$/g of alumina.

<sup>&</sup>lt;sup>3</sup> The AkzoNobel has a TMGa production ability of more than 20 000 kg per year. With their market share, we can obtain that SAFC has 6800 000g/year and Krocera has 13200000g/year.

<sup>&</sup>lt;sup>4</sup> The AkzoNobel has a TMIn production ability of more than 1000 kg per year. With their market share, we can obtain that SAFC has 340 000g/year and Krocera has 660 000g/year.

<sup>&</sup>lt;sup>5</sup> The AkzoNobel has a production ability of more than 5000 kg per year. With their market share, we can obtain that SAFC has 1700 000g/year and Krocera has 3300 000g/year.

<sup>&</sup>lt;sup>6</sup> The Zhuhai Hanbo Trading(2016) is offering a price between 0.5 to 2 \$/g for its product « rare earth YAG yellow led Phosphor ,yellow fluorescent phosphor powder ». We assume that the company is buying with its average price 1.25 \$/kg.

Beijing Yuji Science	CN	33,30%	3476,52	1.65 <sup>8</sup>	25000000 <sup>9</sup>	Yellow phosphor
and Technology Co						
Longkou Unity						
Machinery	CN	33,30%	3476,52	3 <sup>10</sup>	52000000 <sup>11</sup>	Yellow phosphor
Equipement Co						
Jiangsu Plaza						
Premium Electric	CN	33,30%	239,76	91.6 <sup>12</sup>	72000	Gold wire
Instrument						
California Fine Wire	US	33,30%	239,76	91.6 <sup>13</sup>	72000 <sup>14</sup>	Gold wire
Haraeus	GM	33,30%	239,76	91.6	72000	Gold wire
Indium Corporation	US	33,30%	96583,32	9.4 <sup>15</sup>	866 667 <sup>16</sup>	AuSn Solder
Molex	US	33,30%	96583,32	9.4	866 667	AuSn Solder
Lucas Milhaupt						
Global Brazing	US	33,30%	96583,32	9.4	866 667	AuSn Solder
Solutions						

<sup>7</sup> The Zhuhai Hanbo Trading(2016) has a supply ability of 1000 kg per week for its product « rare earth YAG yellow led Phosphor ,yellow fluorescent phosphor powder ».

<sup>8</sup> The Beijing Yuji Science and Technology Co.(2016b) is offering a price between 0.8 to 2.5 \$/g for its product "YAG yellow phosphors". We assume that the company get the average price 1.5\$/g.

<sup>9</sup> The Beijing Yuji Science and Technology Co(YUJI, 2016a, 2016b) has a supply ability of 100 kg/month for 21 yellow phosphors.

<sup>10</sup> The Longkou Unity Machinery Equipement Co. is offering a price between 2 to 4 % for its product "Good quality YAG yellow phosphors for led with CE APPROVED". We assume the company is purchaisng with the average price 3 %.

<sup>11</sup> The Longkou Unity Machinery Equipement Co. has a supply ability of 1000000 g per week for its product "Good quality YAG yellow phosphors for led with CE APPROVED".

<sup>12</sup> The Jiangsu Plaza is offering a price of 0.55\$/m for a minimum order quantity of 2000 meters (Wendy, 2016). With the information that one meter is 0.006g. So the price is 91.6\$/g.

<sup>13</sup> We assume that California Fine Wire and Haraeus offer the same price as Plaza for gold wire.

 $^{\rm 14}$  We assume that California Fine Wire and Haraeus have the same supplying ability of Plaza's.

<sup>15</sup> We assume that the three suplliers of AuSn solder offer the same price as the one got above.

<sup>16</sup> We assume that the three suppliers of AuSn solder has the same supply ability as the estimated from Newsky (Guangzhou Newsky Electronic Co., 2016). Its supply ability is 5000 pcs per week for 100g lead free solder. So its annual supplying capacity is 5000 (pcs/week) \* 52 weeks \* 100 g = 26 000 000 g.

Hunan Jinhao Aluminium Industrial Co.	CN	33,30%	999	0.0052 <sup>17</sup>	8400000 <sup>18</sup>	AI
Zhangqiu Metallic Pigment Co.	CN	33,30%	999	0.0055 <sup>19</sup>	720000000 0 <sup>20</sup>	AI
Chengdu Nuclear 857 New materials Co.	CN	33,30%	999	0.004 <sup>21</sup>	24000000 00 <sup>22</sup>	AI
Zhengzhou Dongyao Nano Materials Co.	CN	33,30%	1318,68	0.55 <sup>23</sup>	52000000 <sup>24</sup>	Ni
Hunan Jinhao Aluminium Industrial Co.	CN	33,30%	1318,68	0.35 <sup>25</sup>	12000000 <sup>26</sup>	Ni
Luoyang Tongrun Info Technology Co.	CN	33,30%	1318,68	0.34 <sup>27</sup>	36000000 0 <sup>28</sup>	Ni

<sup>17</sup> We use the pure aluminium powder. The price is from 4910 to 5500 \$ per ton(Jinhao, 2016). We consider that the company get the average price of 5205\$/ton.

<sup>18</sup> The Hunan Jinhao Aluminium Industrial Co has the supplying ability of 700 kg/month(Jinhao, 2016). We assume that the suppliers (refeining system, Morvillo Precision Product, A metal source) have the same supplying ability.

<sup>19</sup> The Zhangqiu Metallic Pigment Co.(2016) is offering a price between 4 to 7 \$/kg for its product « silver grey pure aluminium powder 99.9 ». We assume that the company is buying with average price 5.5\$/kg.

<sup>20</sup> The supplier Zhangqiu Metallic Pigment Co.(2016) has a supplying ability of 600 tons per month.

<sup>21</sup> The supplier is offering 4\$/kg(Qianwang, 2016) for its product « china Factory-outlet pure aluminum powder ».

<sup>22</sup> The supplier Chengdu Nuclear 857 New materials Co.(2016) has a supplying ability of 2000 tons per months for the « China Factory-outlet pure aluminium powder ».

<sup>23</sup> The Zhengzhou Dongyao Nano Materials Co.(2016) is offering 200 to 900\$/kg for 99.999 nano nickel powder. We assumed that the company is buying with the average price 550\$/kg.

<sup>24</sup> The Zhengzhou Dongyao Nano Materials Co.has a supply ability of 1000 kg per week (2016).

<sup>25</sup> The Hunan Jinhao Aluminium Industrial Co.(2016a) is offering a price form 100 to 600\$/kg for « premium quality 500nano grade nickel powder ».

<sup>26</sup> The Hunan Jinhao Aluminium Industrial Co.(2016a) has a supplying capacity of 1000 kg per month for « premium quality 500nano grade nickel powder ».

 $^{27}$  The Luoyang Tongrun Info Technology Co.(2016b) is offering a price from 2.5 to 669 \$/kg for the its « high purity Ni powder Nano Ni nickel powder ». We assume that the company is buying with the average price 336 \$/kg.

<sup>28</sup> The Luoyang Tongrun Info Technology Co.(2016b) has a suppkying ability of 300 tons per month for the its « high purity Ni powder Nano Ni nickel powder ».

Luoyang Tongrun Info	CN	33,30%	1678.32	0.9 <sup>29</sup>	12000000 <sup>30</sup>	Ag
Technology Co.		,				5
Chengdu Nuclear 857	CN	33 30%	1670 22	0.67 <sup>31</sup>	120000000	۸a
New materials Co.	CN	55,5070	1076,52	0.07	0 <sup>32</sup>	~5
Chengdu Huarui	CN	22 20%	1670.22	1 5 <sup>33</sup>	24000000	٨σ
Industrial Co.	CN	33,3070	10/8,32	1.5	34	Ag
Luoyang Tongrun Info	CN	22 20%	156522.22	0 435	36000000	ті
Technology Co	CN	33,3070	130323,32	0.4	0 <sup>36</sup>	
Changsha Easchem	CN	22 20%	156522.22	<b>n</b> <sup>37</sup>	120000000	ті
Co.	CN	33,3070	150525,52	2	00 <sup>38</sup>	11
Shanghai Ruizheng						
Chemical Technology	CN	33,30%	156523,32	5 <sup>39</sup>	$1000000^{40}$	Ті
Co.						
Luoyang Tongrun Info	CN	22 20%	10090	0.01741	36000000	14/
Technology Co		JJ,JU/0	19990	0.017	042	vv

<sup>29</sup> The Luoyang Tongrun Info Technology Co., Ltd(2016) is offering 300 to 1500 \$/kg for nano silver powder. We assume that the company can get at least 900 \$/kg.

<sup>32</sup> The Chengdu Nuclear 857 New materials Co. (2016a) has a supplying ability of 100 tons per month for its product « Nano silver powder with high purity ».

<sup>33</sup> The Chengdu Huarui Industrial Co.(2016) is offering a price between 1 to 2 \$/g for its product « Nano silver powder ». We assume that the company is buying with the average price of 1.5 \$/g.

<sup>34</sup> The Chengdu Huarui Industrial Co.(2016) has a supplying ability of 20000 kg per month for its product « Nano silver powder ».

 $^{35}$  The The Luoyang Tongrun Info Technology Co(2016c) is offering a price from 300 to 500 \$/kg for its product « Spherical titanium powder ». We assume that the company is buying with the average price of 400 \$/kg.

<sup>36</sup> The The Luoyang Tongrun Info Technology Co(2016c) has a supply ability of 300 tons per month for its product « Spherical titanium powder ».

<sup>37</sup> The Changsha Easchem Co(2016). is offering a price of 1500 to 2500 \$/kg for its product « Titanium nano powder ». We assume that company is buying with the average price of 2 \$/g.

<sup>38</sup> The Changsha Easchem Co. (2016) has a supply ability if 1000 tons per month for its product « Titanium nano powder ».

 $^{39}$  The Shanghai Ruizheng Chemical Technology Co.(2016) is offering a price between 10 to 10 000 \$/kg for its product « Nano titanium powder ». We assume that the compnay is buying with average price of 5005 \$/kg.

<sup>40</sup> The Shanghai Ruizheng Chemical Technology Co.(2016) has a supplying ability of 10000 kg per yea for its product « Nano titanium powder ».

<sup>41</sup> The Luoyang Tongrun Info Technology Co., Ltd(2016a) is offering a price from 1 to 32.21 \$/kg for ultrafine nano tungstun powder high purity nano W tungsten powder. We assume that the company get the average price of 16.6\$/kg.

<sup>&</sup>lt;sup>30</sup> The Luoyang Tongrun Info Technology Co., Ltd(2016) has a supply ability of 1000 kg per month.

 $<sup>^{31}</sup>$  The Chengdu Nuclear 857 New materials Co. (2016a) is offering a price of 674.12 \$/kg for its product « Nano silver powder with high purity ».

Cangzhou Lockeheed Petroleum Machinery Co.	CN	33,30%	19980	0.03 <sup>43</sup>	180000000 44	w
Zhengzhou Dongyao Nano Materials Co.	CN	33,30% <sup>45</sup>	19980	0.5 <sup>46</sup>	52000000 <sup>47</sup>	W

Supplying amount of  $M_i$  from  $S_j$  ( $SA_{(S_j-M_i)}$ ) is the product of supplying ratio  $SR_{(S_j-M_i)}$  and the amount of material  $M_i$  needed to be purchased  $(D_{(M_i)})$ .

<sup>&</sup>lt;sup>42</sup> The Luoyang Tongrun Info Technology Co., Ltd(2016a) has a supply ability of 300 tons per month for ultrafine nano tungstun powder high purity nano W tungsten powder.

<sup>&</sup>lt;sup>43</sup> The Cangzhou Lockeheed Petroleum Machinery Co.(2016) is offering a price between 22 to 38 \$/kg for its product « Nano tungsten powder ». We assume that the company is buying with the average price 30\$/kg.

<sup>&</sup>lt;sup>44</sup> The Cangzhou Lockeheed Petroleum Machinery Co. (2016) has a supply ability of 15 tons per month for its product « Nano tungsten powder ».

<sup>&</sup>lt;sup>45</sup> We didn't find the market share of those suppliers. So we assume that the company is buying equally from these suppliers for the corresponding materirals.

<sup>&</sup>lt;sup>46</sup> The Zhengzhou Dongyao Nano Materials Co.(2016a) is offering a price bewteen 1 to 1000 \$/kg for its product « Nano tungsten podwer ». We assume that the company is buying with the average price 500\$/kg.

<sup>&</sup>lt;sup>47</sup> The Zhengzhou Dongyao Nano Materials Co.(2016a) has a supply ability of 1000 kg per week for its product « Nano tungsten podwer ».

## Relationship with suppliers

Relation with suppliers		Quality of supplying materials	Timeliness	Innovation	Exchange	Human	General score
Sj	L <sub>(Sj)</sub>	$QoM_{S_j}$	$TIM_{S_j}$	Inn <sub>Sj</sub>	Xch <sub>Sj</sub>	$HF_{S_j}$	$QRS_{S_j}$
<b>S1</b>	NL	0,236	0,334	0,648	0,479	0,194	0,535
S2	CN	0,777	0,004	0,048	0,796	0,603	0,611
<b>S</b> 3	US	0,456	0,556	0,073	0,473	0,022	0,608
<b>S</b> 4	CN	0,040	0,533	0,084	0,992	0,316	0,580
S5	CN	0,779	0,563	0,853	0,185	0,295	0,572
S6	CN	0,873	0,714	0,371	0,475	0,621	0,383
S7	CN	0,729	0,900	0,499	0,115	0,795	0,256
S8	CN	0,878	0,679	0,834	0,450	0,059	0,534
S9	KR	0,778	0,078	0,980	0,432	0,594	0,771
S10	GM	0,153	0,905	0,240	0,518	0,097	0,285
S11	CN	0,624	0,104	0,027	0,087	0,439	0,366
S12	US	0,801	0,137	0,768	0,086	0,876	0,704
S13	CN	0,745	0,835	0,510	0,842	0,924	0,508
<b>S14</b>	JP	0,063	0,431	0,445	0,369	0,116	0,671
S15	CN	0,961	0,086	0,004	0,149	0,631	0,459
S16	US	0,981	0,919	0,846	0,665	0,111	0,394
S17	CN	0,897	0,386	0,048	0,609	0,598	0,545
S18	US	0,902	0,699	0,628	0,765	0,360	0,517
S19	US	0,763	0,160	0,474	0,096	0,800	0,342
S20	CN	0,371	0,404	0,977	0,071	0,149	0,634
S21	KR	0,656	0,702	0,789	0,085	0,492	0,535
S22	CN	0,610	0,259	0,900	0,344	0,471	0,611
S23	CN	0,030	0,227	0,188	0,380	0,887	0,608
S24	CN	0,775	0,034	0,627	0,833	0,902	0,580

Table S 39 : Relationship with suppliers (the score of the "quality of supplying material", "time", " Price", "innovtion", "exchange", and "human" are random figures created by Excel)

#### d. Global reserve and production of related mineral elements

Mineral elements	Global reserve	Global production
of materials	2012 (tons)	2012 (tons)
Ag	520000	26000
Al	62900	47600
Au	55000	2800
Ce	Not available	Not available
Ga	Not available	273
In	Not available	799
Ni	8100000	2630000
Sn	4800000	294000
Ti	1120300	209000
W	3300000	81400
Y	540000	7100

Table S 40: Global reserves and production amount of related mineral elements of LED based on (USGS, 2016)<sup>48</sup>

Based on the USGS mineral commodity summaries(USGS, 2015b), the United States and China are the top two producer of rare earth oxide. The U.S had 5 500 tons of rare earth mine production and 1800000 tons of reserve of rare earth oxide in 2013. China had 95 000 tons of rare earth mine production and 55000000 tons of rare earth oxide reserve in 2013. The Lateritic ore in China contains around 10% of Cerium and Bastnasite ore in US containes around 53% of cerium. So the world production of cerium in 2013 was around:

 $5500 \times 53\% + 95000 \times 10\% = 12415$  tons

The world reserve of cerium in 2013 was around:

 $1800000 \times 53\% + 55000000 \times 10\% = 6454000$  tons

 $<sup>^{\</sup>rm 48}$  In the USGS mineral report, the recyclying rate is the secondary production / total production.

#### e. Environment profile

From the database Ecoinvent 2.2, we found the following environmental impact information:

Ecoinvent	2,2	Unit		Method	Method				
Human To:	kicity	kg 1,4	4-DCB-Eq	ReCiPe Mid	ReCiPe Midpoint (E)/human toxicity: 1				
Eco toxicity	/	kg 2,4	4-D-Eq	TRACI/environmental impact: 6 US					8107,7
GWP 100a		kg CC	D2-Eq	EDIP2003 w/o LT/global warming w/o LT: 3 GLO					441,52
Al	Ce	e Ga		In	Ni	Sn	Ti	W	Υ
162,78	3	95,35	1773,6	18579	2992,9	348,33	0,21438	2305,9	4,3496
3,7724	3	95,35	27,512	1697,6	151,82	205,69	0,76478	89,699	15,523
8,3723	1	1,251	203,46	154,28	10,897	17,174	4,5484	446,84	55,497

Table S 41: Environmental impacts of each LED mineral element based on Ecoinvent 2.2

Table S 42: Recycling rate of each mineral element

Mineral elements of	Recycling	Reference
materials	rate	
Ag	47%	(USGS, 2016) <sup>49</sup>
AI	46%	(USGS, 2016)
Au	32%	(USGS, 2016)
Се	0%	(Buchert et al., 2012)⁵⁰
Ga	0%	(Buchert et al., 2012)
In	0%	(Buchert et al., 2012)
Ni	41%	(USGS, 2016)
Sn	60%	(Russell & Lee, 2005)
Ti	24%	(USGS, 2016)
W	53%	(USGS, 2016)
Y	0%	(Buchert et al., 2012)

After combined the percentage of the above mineral element in each material, we obtained the recycling rate value of each material to be analysed as below:

 $<sup>^{\</sup>rm 49}$  In the USGS mineral report, the recyclying rate is the secondary production / total production.

<sup>&</sup>lt;sup>50</sup> Here the 0% means the recyclying is almost zero or less than 1%.

Table S 43: Recycling rate corresponding to materials (based on the percentage of their containing mineral element and element's recycling rate)

Materials	Recycling rate
Ce 3+: YAG (Y3Al5O12(Ce))	8%
TMGa (Ga(CH3)3)	0%
TMIn (InC3H9)	17%
TMAI (C6H18Al2)	17%
Al	46%
Ni	41%
Ag	47%
Ti	24%
W	53%
Alumina	24%
AuSn solder	43%
Gold	32%

For example, the Ce 3+: YAG (Y3Al5O12(Ce)) contains 18.4% of Aluminium, 19.1% of Cerium and 36.4% of Yttrium. So the recycling rate related to Ce 3+: YAG is:

 $Percent \ of \ aluminium \times Recycling \ rate \ of \ aluminium + \ Percent \ of \ cerium$ 

× Recycling rate of cerium + Percent of yttrium

 $\times$  Recycling rate of yttrium =  $18.4\% \times 46\% + 19.1\% \times 0 + 36.4\% \times 0 = 8\%$ 

For example, the Gold wire contains only gold. So the recycling rate corresponding to gold is:

Percent of gold  $\times$  Recycling rate of gold =  $100\% \times 32\% = 32\%$ 

#### f. Legislation profile

Table S 44: Legislation ban or hinder level

	Legislation ban or hinder level note						
Code	Materials element name	Note					
M_1	Ag	0					
M_2	Al	0					
M_3	Au	0					
M_4	Ce	0					
M_5	Ga	0					
M_6	In	0					

M_7	Ni	0
M_8	Sn	0
M_9	Ti	0
M_10	W	0
M_11	Υ	0

### g. Geographic related

From the standards stated in the previous paper, we obtained the following diplomatic score:

Table S 45	: Diplomatic	relations	among	countries
				000

	France	China	Germany	Japan	Korea	Netherland	<b>United States</b>
France	0	0,5	0	0,5	0,5	0	0,5

Table S 46: Bilateral economic exchange between France and other countries (source from (French<br/>Gov., 2015a))

France &	China	Germany	Japan	Korea	Netherland	United States
Export of France / M€	14 740	3 730	6 798	4 242	17 614	26 921
Import of France/ M€	40 830	46 255	8 235	3 887	22 032	32 642
Stock investment of France in the country / M€	18 312	52 774	23 241	3 546	106 583	150 586
Turnover of French companies in the country / M€	49 068	136 450	21 600	7 867	46 000	200 480
Total / M€	122 950	239 209	59 874	19 542	192 229	410 629

Table S 47 : St	tability score	s of supplying	g countries
-----------------	----------------	----------------	-------------

						Nether-	United
	Stability	China	Germany	Japan	Korea	land	States
Original scale							
1-189	Ease of doing business 2014	83	15	30	4	25	7
10-120	Fragile States index (FFP, 2012)	78,3	31,7	43,5	37,6	28,1	34,8

	Estimated political stability by						
(-2,5)-(2,5)	country 2012	-0,54	0,77	0,94	0,17	1,17	0,63
	Worldwide Governance	,	,		,		,
0-100	Indicator	35,1	89,2	85 <i>,</i> 5	72,6	95,8	85,6
	Detemined order: biggier	the valu	ue, worse is	s the sta	bility		
Ease c	f doing business (1 to189)	83	15	30	4	25	7
Fragile Stat	es index (10 to 120) (FFP, 2013)	78,3	31,7	43,5	37,6	28,1	34,8
Estimate	d political stability by country						
(from – 2.5 to 2.5)		0,54	-0,77	-0 <i>,</i> 94	-0,17	-1,17	-0,63
Worldwide Governance Indicator (from 0 to							
	35,1	89,2	85 <i>,</i> 5	72,6	95,8	85,6	
	0-100	scale o	rder				
Ease c	f doing business (1 to189)	43,9	7,9	15,9	2,1	13,2	3,7
Fragile Stat	es index (10 to 120) (FFP, 2013)	61,4	18,2	29,2	23,7	14,9	21,1
Estimate	d political stability by country						
(from – 2.5 to 2.5)		60,8	34,6	31,2	46,6	26,6	37,4
Worldwide	Governance Indicator (from 0 to						
	100)	35,1	89,2	85 <i>,</i> 5	72,6	95,8	85,6
	General score	50,3	37,5	40,4	36,3	37,6	37,0

Table S 48 : Materials supplying amount in corresponding to supplying countries

Materials supplying amount & countries	CN	GM	JP	KR	NL	US
<i>M</i> <sub>1</sub>	10429,56	0,00	0,00	0,00	0,00	0,00
<i>M</i> <sub>2</sub>	0,00	0,00	0,00	485100,00	735000,00	249900,00
$M_3$	0,00	0,00	0,00	3286,80	4980,00	1693,20
$M_4$	0,00	0,00	0,00	990,00	1500,00	510,00
$M_5$	2997,00	0,00	0,00	0,00	0,00	0,00
$M_6$	3956,04	0,00	0,00	0,00	0,00	0,00
<i>M</i> <sub>7</sub>	5034,96	0,00	0,00	0,00	0,00	0,00
<i>M</i> <sub>8</sub>	469569,96	0,00	0,00	0,00	0,00	0,00
$M_9$	59940,00	0,00	0,00	0,00	0,00	0,00
M <sub>10</sub>	7040023,20	0,00	4358109,60	5196207,60	0,00	0,00
<i>M</i> <sub>11</sub>	0,00	0,00	0,00	0,00	0,00	289749,96
M <sub>12</sub>	239,76	239,76	0,00	0,00	0,00	239,76

### **B.** Results presentation



Figure S 2 : Histogram of criticality of materials of LED with contribution score of each criterion with a threshold of 20%, adjusted by exponential function



Figure S 3 : Radar chart criticality conribution with a threshold of 20% and adjusted by exponential function – Group A



Figure S 4 : Radar chart criticality conribution with a threshold of 20% and adjusted by exponential function – Group B



Figure S 5 : Radar chart criticality conribution with a threshold of 20% and adjusted by exponential function – Group C



Figure S 6 : Histogram of criticality of materials of LED with contribution score of each criterion with a threshold of 50%, adjusted by exponential function



Figure S 7 : Radar chart criticality conribution with a threshold of 50% and adjusted by exponential function – Group A



Figure S 8 : Radar chart criticality conribution with a threshold of 50% and adjusted by exponential function – Group B



Figure S 9: Histogram of criticality of materials of LED with contribution score of each criterion with a threshold of 50%, adjusted by arctan function



Figure S 10 : Radar chart criticality conribution with a threshold of 50% and adjusted by arctan function – Group A



Figure S 11 : Radar chart criticality conribution with a threshold of 50% and adjusted by arctan function – Group B

## C. Sensitivity analysis

When a product is determined, the  $M_i$  (including the mineral elements),  $S_j$ ,  $L_{S_j}$ , CL,  $R_{(M_i)}$ ,  $SR_{(S_j-M_i)}$ , and one product's mass are constant.

List of inputs:

When:

Then

 $x1_{M_i} = value of selected environmental indicator$ 

 $y_{M_i} = C4$ 

When:

Then

$$x2_{M_i} = recycling \ rate \ of \ material$$

 $y_{M_i} = C12$ 

When:

 $y_{M_i} = C8$ 

Then

```
x3_{M_i} = global production amount of material
x4_{M_i} = global reserve amount of material
```

When:

$$y_{M_i} = C1$$

Then

$$x5_{M_i}$$
 = accessible supplying amount of material  
 $x6_{M_i}$  = planned purchase amount of material

When:

$$y_{M_i} = C2$$

Then

$$x_{6M_i} = planned purchase amount of material$$
  
 $x_{7M_i} = function value of material$   
 $x_{8M_i} = Price$   
 $Z_{1M_i} = Supplying ratio of each supplier SR_{(S_j - M_i)}$ 

When:

$$y_{M_i} = C7$$

Then

$$x9_{M_i}$$
 = relation score with each supplier  
 $Z1_{M_i}$  = Supplying ratio of each supplier  $SR_{(S_j-M_i)}$   
 $Z2_{M_i}$  = Suppliers  $S_j$ 

When:

$$y_{M_i} = C11$$

Then

$$x10_{M_i} = stability \text{ or ease of doing business}$$
  
 $Z1_{M_i} = Supplying \text{ ratio of each supplier } SR_{(S_j - M_i)}$   
 $Z2_{M_i} = Suppliers S_j$   
 $Z3_{M_i} = Supplying \text{ country } L_{S_j}$ 

When:

$$y_{M_i} = C9$$

Then

$$x11_{M_i} = sgeo relation between supply country an buy country$$
  
 $x12_{M_i} = economic bilateral exchange between supply country and buy country$   
 $Z3_{M_i} = Supplying country L_{S_j}$ 

The inputs are considered stable.

List of outputs

For  $M_i$ ,  $y_{M_i} = (C1_{M_i}, C2_{M_i}, C4_{M_i}, C6_{M_i}, C7_{M_i}, C8_{M_i}, C9_{M_i}, C11_{M_i}, C12_{M_i}, C_{M_i})$ 

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# **RÉSUMÉ EN FRANÇAIS**

### Introduction

Le développement de la société et de la technologie demande de plus en plus de ressources pendant que la globalisation rend possible l'accès à plus de matériaux partout dans le monde. Pourtant, l'approvisionnement de ces ressources ne peut pas toujours satisfaire la demande. Ces matériaux peuvent être très importants ou irremplaçables pour certaines entreprises ou pays dans certains moments. Une perturbation peut avoir une influence énorme sur les secteurs concernés pouvant même mener à des crises ou conflits pour des matériaux. Par exemple, une crise liée au cobalt a eu lieu à la fin des années 1970 stimulée par la guerre civile au Zaïre qui produisait la majorité du cobalt à ce moment ; un conflit lié au palladium a eu lieu dans les années 1990 à cause de l'arrêt d'exportation par la Russie ; des chocs pétroliers sont apparus en 1973 et 1979 à cause des limitations d'exportations imposées par les pays arabes aux pays qui supportaient Israël et une crise des terres rares (une famille de métaux) a eu lieu en 2010 à cause des politiques d'exportation de la Chine qui produit 97% des terres rares à ce moment. Dans le même temps, ces crises peuvent gravement endommager ou affecter les industries, l'économie ou la sécurité des pays concernés. L'usage du mot « criticité » est récent pour interpréter ce genre de phénomène. En dehors des causes directes mentionnées précédemment, ces crises sont liées à l'interaction de divers autres paramètres. Par conséquent, il est important de comprendre le mécanisme de la criticité afin de nous aider à mieux nous préparer face à ces crises ou même à les éviter.

Le but de cette thèse est de comprendre la criticité des matériaux et de savoir comment la déterminer au niveau du produit. Les objectifs sont les suivants :

- Établir un diagramme général qui représente le domaine de recherche de la criticité.
   Étudier l'histoire de ce domaine pour savoir ce qui a été fait (comment les autres chercheurs interprètent la criticité, dans quelles conditions, comment ils l'évaluent etc.) et ce qui doit être fait.
- ii. Déterminer les paramètres qui influencent la criticité des matériaux.
- Définir la criticité des matériaux. Avant de proposer une définition, une bonne compréhension du mécanisme de la criticité, y compris les paramètres qui rendent les matériaux critiques et des conditions, est nécessaire.

iv. Développer une méthodologie d'évaluation de la criticité des matériaux au niveau du produit.

# État de l'art

L'état de l'art primaire est basé sur 48 études datées de 1974 à 2014. Les études examinées viennent des bases de données scientifiques, de documents gouvernementaux ou professionnels, de moteur de recherche et de la bibliothèque de l'université. Elles se présentent sous formes de projets d'acte du gouvernement, livres, articles de journaux, magazines, rapports, mémoires de thèse, mémoires de master etc. Les articles de journaux viennent de journaux anglais suivants : "Resources, conservation and recycling", "Resources Policy", "Renewable and Sustainable Energy Reviews", "Environment Science & Technology", "Applied Energy", "Ecological Economics", and "Science of total environment". Le magazine pris en compte est le "Mechanical Engineering Magazine". Du fait que certaines études sont confidentielles ou rédigées dans une langue que l'auteur ne maîtrise pas, cet état de l'art ne peut pas couvrir toutes les études sur la criticité. De plus, avec la limite de temps et des moyens de recherche, il est une bibliographie non-exhaustive. Certaines ressources sont ajoutées au fur et à mesure de la réalisation de la thèse. A la fin, parce que certains travaux liés à la disponibilité, la rareté et au risque d'approvisionnement des matériaux sont similaires à ceux de la criticité, ils ont été inclus dans cet état de l'art.

Le mot « critique » est apparu en premier dans un protocole d'accord américain en 1974 qui sert à diriger les stratégies nationales des produits de base hors combustibles importés (The White House, 1974). 34 ans plus tard, une matrice de la criticité qui sert à déterminer la criticité des matériaux a été inventée dans une étude réalisée par le National Research Council (2008). Cette matrice est devenue le concept de base de nombreuses études ultérieures y compris deux études connues de 2010 : celle de la Commission Européenne et celle du Département de l'Énergie. En ce moment, il n'y a pas de définition consensuelle de la criticité (Lloyd et al., 2012) ou de méthodologie d'évaluation. Huit versions de la définition de la criticité sont extraites des études examinées. Après avoir comparé leurs mots clés, nous pouvons voir que « l'approvisionnement » (y compris le risque d'approvisionnement, la restriction de l'approvisionnement, etc.) a été mentionné huit fois sur huit, suivi des mots clés comme «demande », « importance », « fonction », et « substitution » qui sont mentionnés 2

fois sur 8. Les mots clés suivants sont mentionnés une fois : « impact », « environnement », « indisponibilité » et « haut prix ». Deux définitions ont même spécifié la condition : l'urgence nationale (96th congress, 1979) et l'énergie / les nouvelles technologies émergentes (APS & MRS, 2011). Même s'il n'y a pas encore de consensus, la majorité des organisations ou chercheurs européens acceptent davantage la définition proposée par la Commission Européenne. La méthodologie proposée par l'Université de Yale adopte plutôt la définition du National Research Council (2008) en ajoutant l'aspect environnemental.

Parmi ces 48 études, 48% sont conduites par des instituts américains et 44% sont réalisées par des organisations ou chercheurs européens. A part l'Union Européenne et les Etats-Unis, le Japon a aussi lancé des recherches dans ce domaine. Il convient de mentionner que ces trois acteurs sont aussi ceux qui ont lancé une plainte contre la Chine auprès de l'Organisation Mondiale du Commerce concernant les terres rares. Nous pouvons donc faire l'hypothèse que les pays développés qui sont plus avancés dans le domaine des hautes technologies et qui dépendent des ressources importées sont plus sensibles à la criticité des matériaux. De plus, plus de la moitié de ces études sont réalisées par des instituts de recherche ou des universités et un tiers sont conduits par des organisations gouvernementales. Cependant, en dehors des études faites par l'Université de Yale et des mémoires de thèses ou master, la plupart des études faites par les instituts de recherches sont aussi liées aux besoins gouvernementaux.

Concernant les matériaux étudiés ou désignés critiques dans ces études, certaines désignent directement des matériaux critiques sans les comparer à d'autres candidats et sans processus d'évaluation. Parmi les 80 matériaux étudiés en plus du groupe Platinum et des terres rares, la majorité sont de métaux (40 éléments). Le reste des matériaux couvert sont des éléments nonmétaux, des métalloïdes, des composés, et même des ressources organiques. Les matériaux suivants sont ceux qui ont été le plus fréquemment mentionnés : le gallium, l'indium, le cobalt, le tellure, le germanium, le niobium et des terres rares. Même certains matériaux très répandus dans la croûte terrestre sont étudiés tel que la silicone. Certains matériaux de production massive sont aussi étudiés, tels que le cuivre, l'acier, etc. Les matériaux désignés critiques sont regroupés dans trois catégories en fonction de leurs usages (dans l'ordre de fréquence du matériau le plus cité au moins cité) : Technologies propres (Indium, Néodyme, Gallium, Dysprosium, Tellure, Germanium, etc.). Sécurité nationale (Aluminium, Chrome, Manganèse, Antimoine, Béryllium, Bismuth etc.) et Economie générale (Magnésium, Indium, Néodyme, Aluminium, Antimoine, Cobalt, etc.).



Figure 2 : Concepts basiques appliqués dans les études examinées

Parmi les études qui ont développé des méthodologies d'évaluation, quatre concepts de base sont extraits (figure 2) : le modèle cartésien à deux dimensions (National Research Council, 2008), le modèle cartésien à trois dimensions (Yale University), le modèle à trois cercles (Öko-Institut, 2009) et la carte radar à cinq dimensions (Claire, 2011). Les dimensions (critères généraux) d'évaluation sont similaires aux mots clés des définitions : demande, approvisionnement, vulnérabilité face au risque d'approvisionnement, environnement, importance / impact, recyclage, matériaux et innovation. Il existe neuf combinaisons de ces dimensions pour évaluer la criticité dont quatre contiennent deux dimensions et cinq contiennent trois dimensions. La dimension « approvisionnement » est aussi celle qui a été pris en compte dans toutes les méthodologies en dehors celle de Bachér et al. (2013) qui a considéré « l'environnement », «l'importance / impact » et « l'innovation ». Les combinaisons entre les dimensions « approvisionnement », « importance / impact », « demande » ou « environnement » sont les plus fréquentes.

Les sources de données que ces méthodologies utilisent sont regroupées dans la table 5, par exemple, les United States Geographical Surveys (USGS) pour les données de production ou réserve, la World Bank (Banque Mondiale) pour les données interdisciplinaires etc.



Figure 3 : Diagramme sur le domaine de recherche de la criticité

A la fin, la figure 3 conclut le domaine de recherche de la criticité. En général, quand nous conduisons une étude de la criticité des matériaux, le but est de trouver des solutions ou des mesures de prévention afin de soulager ou prévenir les problèmes causés par les matériaux

critiques. Ce but est désigné comme la phase finale d'une étude de la criticité. Pour atteindre ce but, nous devons savoir quels matériaux sont critiques et en quoi sont-ils critiques. C'est aussi la phase où une méthodologie ou un modèle d'évaluation quantitative est demandé. Cette partie est désignée comme la phase intermédiaire. Afin de développer la méthodologie ou le modèle d'évaluation, nous devons savoir quels paramètres influencent la criticité des matériaux et le mécanisme. Cette partie est appelée la phase première ou la phase de diagnostic. Les étapes ci-dessus représentent le fil de la pensée quand nous sommes face au problème de la criticité. En revanche, pour atteindre la phase finale, l'ordre de mise en place de la recherche sur la criticité est de commencer par la phase de diagnostic, puis de développer la méthodologie et finalement de proposer des solutions ou mesures d'atténuation. Cependant, la plupart des études examinées commencent directement par développer des méthodologies sans la phase de diagnostic de la criticité ou sans un diagnostic compréhensif (qui est disponible au public). À l'heure actuelle, il existe des méthodologies pour évaluer la criticité des matériaux au niveau d'une région administrative (European Commission, 2010, 2014), pour les technologies (Department of Energy 2010, 2011), et pour un ensemble de métaux spécifiques (Graedel et al., 2012) (Harper et al., 2015). Ces études ont été regroupées dans la phase intermédiaire. Néanmoins, ces résultats ne peuvent pas être directement utilisés par les industries pour les raisons suivantes : 1) les portées sont différentes (les objectifs de l'entreprise / préférences, les échelles, les facteurs géographiques etc.) ; 2) les matériaux de base sont différents, des matériaux indiqués critiques dans des études précédentes ne sont parfois même pas connectés aux activités de cette industrie spécifique. Certaines études ont travaillé sur des solutions plus détaillées avec des résultats issus d'études précédentes. Par exemple, Statistics Netherlands (2010) a analysé l'influence des matériaux déterminés critiques par la Commission Européenne sur les industries néerlandaises. Rademaker et al (2013) s'est concentré sur les approches d'atténuation face à la criticité des terres rares. Ces études ont été regroupées dans la phase finale. Basées sur cet état de l'art, trois lacunes de recherche ont été identifié : 1) il manque un diagnostic compréhensif de la criticité (première phase) ; 2) il manque une méthodologie d'évaluation au niveau du produit ; 3) il manque des liens entre les différentes phases.

## Diagnostic de la criticité

Basé sur l'état de l'art, il est important de d'abord réaliser un diagnostic de la criticité et ceci reste encore une partie peu travaillée. Cette partie vise à éliminer la première lacune et à servir comme noyau de recherche pour le reste du projet.



Figure 4 : Méthodologie de recherche sur le mécanisme de la criticité (nommé comme le diagnostic)

La méthodologie de recherche pour le diagnostic est illustrée dans la figure 4. La première étape est de chercher des informations y compris les définitions des mots suivants : critique, stratégie, important. Ceci permet de donner une idée générale de la criticité. La deuxième étape est de réaliser un état de l'art sur les études existantes concernant les matériaux critiques. Cela sert à savoir comment la criticité a été interprétée et évaluée jusqu'à maintenant ainsi qu'à acquérir des connaissances plus profondes et concrètes sur la notion de criticité. La troisième étape est de poser une question « quels paramètres peuvent influencer la criticité des matériaux au niveau du produit ? ». Cette question sert de ligne directrice pour les

réflexions dans les étapes suivantes. La quatrième étape est de déterminer les critères-clés de la criticité à l'aide des trois étapes précédentes. La cinquième étape est d'établir une forme embryonnaire du mécanisme de la criticité. La sixième étape est de se pencher sur des indicateurs quantitatifs ou qualitatifs mentionnés dans les études examinées afin de voir s'ils peuvent être ajoutés dans le diagramme primaire du mécanisme. La septième étape est de faire une réflexion finale / brainstorming pour des paramètres d'impact de la criticité dans les aspects suivants : technologique, sociale, économique, politique, géographique et environnemental. Cette étape sert à renforcer le diagramme du mécanisme. La huitième étape est d'établir le mécanisme complet des paramètres d'impact de la criticité.



Figure 8 : Paramèters d'impacts issue de la partie diagnostique

À la suite de cette méthode de recherche, les résultats du diagnostic sont présentés dans la figure 8. Dans l'ensemble, la criticité des matériaux au niveau du produit est influencée par quatre dimensions : l'importance des matériaux, l'accessibilité de l'approvisionnement, le déséquilibre entre la demande et l'approvisionnement ainsi que les aspects dynamiques ou des changements brusques.

Plus précisément, la première dimension est l'importance des matériaux pour le produit que l'acteur veut analyser. Cette dimension contient les branches suivantes : la fonctionnalité, la substitution et l'influence économique. D'un côté, la fonctionnalité représente l'importance fonctionnelle que ces matériaux offrent au produit, elle peut être liée avec certaines propriétés des matériaux. Quand un matériau est requis, c'est plutôt pour ses fonctionnalités que pour le matériau lui-même. Ce n'est pas non plus pour d'autres fonctionnalités possédées par ce matériau qui n'ont pas de relation avec la fonctionnalité attendue. D'un autre côté, si ce matériau peut être remplacé par d'autres qui répondent à tous les critères, il est considéré peu important pour ce produit. Enfin, l'influence économique représente l'importance du coût de ce matériau pour l'industrie. Ceci a été inspiré par l'attitude de l'industrie pétrolière face à l'augmentation du prix des terres rares en 2010. Bien que le prix des terres rares ait beaucoup augmenté et qu'il existe des substituts qui peuvent aussi être utilisés comme catalyseurs, l'industrie pétrolière a continué d'utiliser les terres rares car l'augmentation du prix des terres rares rares rares rares rares influence très peu le coût final du pétrole.

La deuxième dimension, l'accessibilité à l'approvisionnement, peut être divisée en deux parties : l'approvisionnement auquel nous n'avons pas accès et l'approvisionnement auquel nous ne devons pas avoir accès. La raison de cette différenciation est liée au fait que les solutions associées soient différentes. C'est pour faciliter l'automatisation du travail concernant la troisième lacune (l'établissement des liens entre les différentes phases) dans le futur. Par exemple, le mercure est interdit dans la production de lampes. Dans ce cas-là, nous devons chercher d'autres substituts plutôt que faciliter l'accessibilité au mercure. La partie concernant « l'approvisionnement auquel nous n'avons pas accès » peut être divisée en causes venant des fournisseurs et de l'entourage. Concernant les fournisseurs, les paramètres considérés sont la diversité des fournisseurs, leurs locations, les relations entre l'industrie (l'acteur qui conduit l'étude de la criticité) et ses fournisseurs, les prix d'achat, les problèmes

internes des fournisseurs etc. En termes d'entourage, les paramètres considérés sont la compétition venant d'autres secteurs surtout la défense, la dépendance du secteur des matériaux analysés envers les autres marchés, les réserves globales, la géo-relation (politique et économique) entre le pays des fournisseurs et le pays de l'industrie, la stabilité des pays des fournisseurs, les restrictions venant des pays des fournisseurs (par exemple la priorité de satisfaire aux besoins internes dans les pays des fournisseurs, les manifestations, des changements des lois etc.), le rapport entre la demande et l'approvisionnement mondial et le taux de recyclage de ce matériau.

La troisième dimension est le déséquilibre entre la demande dont une industrie spécifique a besoin pour la production de son produit et l'approvisionnement auquel l'industrie peut accéder. Industrie spécifique (l'acteur) indique ici que cette interprétation considère les différentes conséquences venant de différents acteurs. La raison pour combiner la demande et l'approvisionnement est que ce ne sont pas deux facteurs influençant indépendamment la criticité des matériaux mais davantage leurs rapports.

La quatrième dimension, le facteur dynamique ou changement brusque, est la seule dimension qui ne peut pas être évaluée directement. Le fait que la situation change brusquement est parfois plus dérangeant que la situation elle-même. En réalité, le marché répond lui-même aux problèmes liés à la criticité, un matériau ne peut donc pas être critique pour toujours. Par conséquent, le temps que l'acteur utilise pour s'adapter à la nouvelle situation est vitale. Si ce temps est inférieur au temps dont le marché a besoin pour atteindre son nouvel équilibre, l'acteur survit. Dans le cas contraire, l'acteur devra en subir les conséquences. La criticité varie en fonction des différentes périodes ou des différentes situations. Les facteurs dynamiques incluent : qui, quoi, quand, où et pourquoi. « Qui » représente l'acteur qui conduit l'étude de la criticité. « Quoi » représente le sujet (un produit, une technologie, un pays etc. dans les études examinées) que l'acteur veut analyser. Ces « qui » et « quoi » peuvent être définis pendant l'établissement du périmètre de l'étude. « Quand » représente le temps, y compris les situations en ce moment, le temps (durée) que le sujet exige pour réagir et le temps (durée) que le marché a besoin pour réagir. Le « Quand » peut être concrétisé par la sélection des données (actuelles, passées, ou dans un temps spécifique) des indicateurs qui évoluent dans le temps ainsi que des scénarios. « Où » représente l'aspect géographique comme les pays ou les régions des acteurs concernés par le scénario (où se situe le sujet, où se

situent ses fournisseurs, où se situent les réserves etc.). « Où » peut être exprimé par des indicateurs liés à l'aspect géographique des régions telles où les réserves de matières premières sont présentes et exploitées, des lieux où se situe chaque fournisseur, etc. « Pourquoi » représente les aspects jugés importants lors de l'étude de la criticité. Ce « pourquoi » est défini par la description du scénario ou les lignes directrices établies lors de l'établissement du périmètre de l'étude. En générale, l'approche utilisée pour cette dimension est de l'intégrer dans les autres indicateurs qui impliquent déjà un aspect dynamique dans leurs natures ou évoluent dans le temps (Komal, 2015) et dans la structure de la méthodologie tels que l'établissement du scénario, du périmètre de l'étude, etc. Ces facteurs dynamiques servent aussi à connecter les autres paramètres d'impact correspondants.

Finalement, voici la définition proposée : la criticité des matériaux est une valeur relative à l'interaction entre l'importance des matériaux considérés pour l'application, le déséquilibre entre la demande et l'approvisionnement, et l'accessibilité à l'approvisionnement. La criticité est renforcée par les changements brusques ou les situations où l'acteur ne peut pas s'adapter à temps.

Tous les matériaux sont plus ou moins importants selon les cas. L'aspect relatif de la définition souligne que l'importance des autres matériaux n'est pas ignorée mais seulement que ceux qui exigent un intérêt particulier sont mis en avant. L'application mentionnée dans la définition fait aussi référence au facteur dynamique « quoi » défini précédemment : l'application pour laquelle l'acteur veut analyser la criticité des matériaux, comme un produit, une technologie, un groupe de matériaux, ou un pays. Le fait d'exprimer la situation particulière en précisant les termes ci-dessus est un moyen de projeter le concept dynamique de la criticité.

## Étude de cas des terres rares

La raison de faire une étude de cas compréhensive sur les terres rares tient dans la crise des matériaux la plus récente et celle qui a accéléré la recherche sur la criticité. Les objectifs de cette étude de cas sont de mieux comprendre le mécanisme de la criticité, de chercher des références pour définir et déterminer la criticité et de connaître les influences de cette crise. Ceci sert également comme un complément du diagnostic.

Les matériaux des terres rares concernent les formes suivantes ; les mines, les oxydes, les métaux, les alliages, les semi-produits ou les composants qui contiennent les éléments des terres rares. Les éléments des terres rares incluent 17 éléments métalliques: Scandium (Sc), Yttrium (Y), Lanthane (La), Cérium (Ce), Praséodyme (Pr), Néodyme (Nd), Prométhium (Pm), Samarium (Sm), Europium (Eu), Gadolinium (Gd), Terbium (Tb), Dysprosium (Dy), Holmium (Ho), Erbium (Er), Thulium (Tm), Ytterbium (Yb) et Lutétium (Lu). Du fait que les structures atomiques de ces éléments sont très proches, par exemple elles ont des différences très minimes de leurs niveaux d'électrons et de leurs rayons ioniques. Ces éléments ont des propriétés assez similaires et il est difficile de les séparer au cours de l'exploitation ou du recyclage. C'est pourquoi le substitut d'un élément terre rare vient souvent de la famille des terre rares. Les éléments de terres rares avec les valences +2 ou +4 possèdent des propriétés spécifiques qui peuvent être utilisés dans les semi-conducteurs, les amants et les matériaux luminescents. Les usages des terres rares sont étroitement liés à leurs propriétés. Pour leur fin de vie, le taux de recyclage est moins d'1% à cause de la faible quantité qu'ils contiennent dans les produits, de la difficulté de démonter des produits qui les contiennent, de la difficulté de séparation entre ces éléments et l'immaturité des secteurs liés aux processus du recyclage.

Selon les données de l'USGS, les mines ou les gisements des terres rares ont été découverts partout dans le monde, sauf en Arctique et en Antarctique. Nous avons même découvert les terres rares sur la Lune. Sur Terre, les gisements sont légèrement plus concentrés le long des côtes des continents. Il y a plus de gisements sur les côtes-est du continent Asiatique et de l'Amérique du Sud qui ont été découverts que sur leurs côtes-ouest. L'abondance relative des éléments des terres rares dans la croûte continentale supérieure de la Terre est plus élevée que celles des éléments suivants : Hg, Ag, In etc. De plus, il existe aussi des ressources marines des terres rares et d'autres qui ne sont pas encore découvertes. Pour conclure, les terres rares ne sont pas rares. Parmi les pays où les réserves sont découvertes, la Chine, les États-Unis et la Communauté des Etats indépendants (CIS) sont les trois entités politiques qui possédaient le plus de réserves entre 1995 et 2012. Au Brésil, une grande quantité de réserve des terres rares a été découverte en 2012 dont la proportion a dépassé celle des Etats-Unis. Néanmoins, la Chine domine la production des mines d'oxydes de terres rares depuis 1995. Avant la Chine, les Etats-Unis étaient le pays dominant dans cette activité. Ce déplacement du centre

de gravité a eu lieu en raison du coût de mains d'œuvre, du coût des mines, des pollutions causées par les activités de mines, des oppositions sociales, ainsi que des avantages comparatifs.

Cependant, même si la production augmentait chaque année, le montant de réserve mondiale restait le même ou même augmentait, sauf en 2002. Le montant de la production est très faible comparé avec celui de réserve. En 1998, le montant de réserve était 1600 fois plus important que celui de la production. La réserve mondiale reste au moins 600 fois plus grand que la production. Si la situation reste la même y compris les développements des nouvelles technologies et les découverts des nouveaux gisements, nous pouvons prédire que la réserve pourra satisfaire la demande pour longtemps. Une autre méthode est de considérer la production et la réserve proposée par cette thèse au ratio du pays. C'est-à-dire de regarder la construction de chaque pays dans l'activité de production en fonction de son ratio de réserve. Auprès du calcul, la Malaisie, la Chine et l'Inde sont les trois pays qui produisent le plus comparé avec leurs proportions de réserve dans le monde. CIS et les Etats-Unis sont deux entités politiques qui ont un grand potentiel de production.

La Chine est le pays dominant dans la production des mines des terres rares, elle exportait au moins 44 000 tonnes de produits entre le 1996 et 2009. Son montant d'import reste inférieur à 10 000 tonnes. D'un autre côté, les Etats-Unis importent plus que ce qu'ils exportent. La différence entre l'export et l'import est plus petit que celle de la Chine. Mais les terres rares que la Chine exporte sont souvent des ressources premières et ce qui implique moins de technologies. Elle import les produits des terres rares qui implique plus de hautes technologies. Au contraire, le Japon, les pays européens etc. importent souvent des matières premières des terres rares, les manufacturent puis exportent des produits qui contiennent des éléments terres rares ou des semi-produits des terres rares qui demandent de hautes technologies.

Les politiques chinoises étaient un des enjeux importants de la crise des terres rares récente. Pourtant, si nous prenons en compte toutes les politiques concernées, nous pouvons trouver des indices que la Chine a déjà commencé de mettre en place les politiques plus restrictives sur l'export des terres rares beaucoup plus tôt que l'année 2010. Par exemple, la première politique sur le quota d'exportation a été délivrée en 1999. Et le remboursement des taxes d'exportation s'est rétrécit ou a même été annulé depuis 2004. Les raisons de ces politiques protectives sont : 1) des lourdes pollutions causées par des activités liées à l'exploitation et la manu-facturation des terres rares ; 2) l'épuisement de ressources des terres rares du fait que la réserve des terres rares a diminué de 85% à 36% depuis l'année 1992 au 2009. De plus, le public chinois est plus sensible aux problèmes environnementaux qui engendrent une pression sociale. En Chine, il existe des mines illégales ou privées avec une très faible efficacité ce qui gaspille énormément de ressource. Il existe aussi de la contrebande et la revente de quota pour lutter contre la réduction d'exportation. Même si la technologie chinoise a beaucoup avancé depuis qu'elle a découvert des réserves de terres rares, ses activités dans ce domaine restent encore en amont de la chaine qui est équivalente aux faibles valeurs ajoutées (faible profit). La Chine essaye donc de réformer et revaloriser ces secteurs en changeant les politiques.

La crise des terres rares se réfère à la perturbation de l'approvisionnement lié à une forte augmentation du prix voir même à une interruption de deux mois au Japon en 2010. Dans la même année, les terres rares sont considérées comme des matériaux critiques par la Commission Européen et le Département de l'Energie. C'est aussi l'année où la tension du conflit territoriale du Diaoyu / Senkaku entre la Chine et le Japon était élevée. En 2012, les Etats-Unis ont lancé une plainte à l'Organisation Mondiale du Commerce contre la restriction de l'exportation de la Chine sur certains matériaux y compris des terres rares, rejoints par 18 autres pays.

À la fin, cette étude de cas a servi à compléter et approuver le diagnostic de la criticité. Premièrement, les fonctions que les terres rares offrent sont importantes et même irremplaçables pour certains secteurs ou pays. Ces fonctions sont liées aux propriétés de ces matériaux. L'approche des secteurs pétroliers concernant l'usage des terres rares comme des catalyseurs face à la crise montre l'importance d'ajouter l'influence économique comme un paramètre d'impact. Deuxièmement, même si la demande mondiale des terres rares était assez faible comparée à celles des autres matériaux tels que l'aluminium ou l'acier, l'approvisionnement que certains pays pouvaient avoir était plus faible ou même quasiment nul. C'est le rapport entre la demande et l'approvisionnement qui influence la criticité au lieu de ces deux facteurs individuels. Troisièmement, l'accessibilité à l'approvisionnement des terres rares qui suivent : 1) des fournisseurs qui avaient une très faible diversité (la Chine était le pays qui

fournissait 97% de matières premières des terres), avaient augmenté le prix et avait mis le quota d'exportation et 2) de l'entourage. Par exemple la coupure de deux mois aux industries japonaises ont été causé par la relation géopolitique entre le fournisseur (la Chine) et leur pays (le Japon) selon un directeur japonais d'une société de négoce de matériaux (Ramzy, 2013). Et le taux de recyclage des terres rares était quasiment égal à zéro, même pour le Japon qui possède une énorme mine urbaine qui contient des terres rares. Quatrièmement, c'était une crise brusque pour des pays ou des secteurs concernés n'étaient pas prêts. Par exemple, les nouvelles sources d'approvisionnement n'étaient pas suffisantes. Cela prend du temps pour ouvrir de nouvelles mines ou de trouver des substituts. Le stock n'était pas suffisant. Finalement, le fait que la crise n'a pas touché tous les pays / secteurs et que les différents pays / secteurs ont eu un degré de dommage différent a montré l'importance de souligner le rôle « sujet » et « acteur » en termes de la criticité.

#### Développement de la méthodologie

Dans cette thèse, une méthodologie générale qui vise à évaluer la criticité des matériaux au niveau du produit a été développée et un modèle d'évaluation basé sur un scénario basique a été présenté en détail.



Figure 19 : Lignes directrices de la méthodologie développée

Les processus de la méthodologie sont illustrés par la figure 19. Les lignes directives de la méthodologie sont : 1) Décider du produit cible. Quand le produit cible a été déterminé, tous les matériaux liés sont aussi déterminés, ainsi que les fonctionnalités demandées, le lieu de production, la demande des matériaux liée à la production de ce produit, etc. 2) Décider du groupe de matériaux à analyser. Cette étape est à réduire le nombre des matériaux à analyser. Il est possible que beaucoup de matériaux, directs ou indirects, puissent être liés au produit cible. Avec la limite des ressources ou du temps, nous n'avons parfois pas le choix de filtrer et sélectionner juste une partie des matériaux pour analyser leurs criticités. Cette sélection peut être produite à l'aide d'un travail empirique ou l'expertise. C'est aussi la première fois que la subjectivité a été amenée dans cette méthodologie. 3) Construire le scénario spécifique pour cette étude. Le scénario est un moyen qui permet d'assembler des stratégies de l'entreprise ou différentes possibilités de situation et de les projeter dans les étapes suivantes. Par exemple, le scénario peut être basé sur les données historiques, les données actuelles ou les données prédites. Nous pouvons même établir les situations potentielles puis analyser la criticité dans ces situations. Nous pouvons aussi souligner la préférence stratégique tels que l'innovation, l'environnement, l'économie, etc. Par exemple, quand l'économie de l'entreprise affiche de bons résultats, qu'elle veut favoriser une image pro-environnementale. Il est possible de mettre moins de poids sur les paramètres liés à l'économie et ajouter le poids sur ceux qui sont liés à l'environnement. L'établissement du scénario contient aussi la sélection des paramètres d'impact. Selon la partie diagnostic, nous voyons que de nombreux paramètres d'impact ont été proposés. C'est pendant cette étape que nous sélectionnons ceux qui sont les plus importants et possibles d'être évalués. C'est aussi la deuxième fois que la subjectivité agit dans la méthodologie. 4) Sélectionner les indicateurs pour certains paramètres. Pour certains paramètres, il existe plus d'un seul indicateur d'évaluation. Par exemple, nous avons les indicateurs disponibles tels que l'écotoxicité, le potentiel de réchauffement planétaire etc. pour évaluer les impacts environnementaux d'un matériau. Cette étape permet de choisir ce qui correspond mieux au scénario. Une autre raison d'ajouter cette étape est de permettre à la méthodologie de s'adapter aux nouvelles situations ou aux cas spécifiques même si les méthodes d'évaluations sur certains paramètres évolueront. 5) Entrer ces informations dans le modèle d'évaluation. La méthodologie inclut un modèle d'évaluation qui contient tous les calculs. Les informations des quatre étapes précédentes sont aussi là pour former ce modèle de calcul. 6) Le modèle produit une liste de données nécessaires pour le calcul. L'idée est que le modèle complet contienne toutes les possibilités de calculs ou il est possible d'ajouter de nouveaux calculs. Les calculs sont prévus d'être automatisés sous les outils tels qu'Excel, un site ou un logiciel. De ce fait, une liste de données que nous devons acquérir sera générée automatiquement par le modèle complet. 7) Entrer ces données y compris les poids. C'est aussi l'étape qui prend le plus de temps dans toute la méthodologie. Puis nous devons entrer les données dans le modèle selon la demande. 8) Le modèle génère trois sortes de résultats. Les outputs contiennent un score général de la criticité pour chaque matériau, un diagramme qui montre comment la criticité contribue aux mesures suggérés pour modérer la criticité. Le score général est un résultat qui assemble les différents « critères ». Le diagramme montre aussi les notes de chaque critère pour chaque matériau (exemple disponible à la figure 30 et 31). Concernant les recommandations des approches d'atténuation, une base de données de toutes les mesures d'atténuation qui sont recommandées ou appliquées par des études de criticités existantes doit être établie d'abord. Puis elles sont groupées sous les mots clés des critères ou des paramètres d'impact. En considérant la contribution de chaque critère, ces mesures peuvent être extraites de la base de données

La criticité est évaluée quantitativement et représentée par des « critères » dans le modèle de calcul. La raison de différencier ces critères et ces paramètres d'impact est de faciliter la personnalisation du modèle et de rendre possible l'adaptation de la méthodologie aux différentes situations. Plus précisément, un critère peut contenir plusieurs paramètres d'impact et un paramètre d'impact peut être impliqué dans plusieurs critères. Par exemple, le paramètre d'impact « rapport d'approvisionnement d'un fournisseur » influence les critères « qualité de la relation avec des fournisseurs » et « Géo-relation ». Mais ce paramètre d'impact seul n'est pas approprié pour évaluer la criticité, c'est pourquoi il a été intégré avec d'autres paramètres pour devenir un critère qui peut évaluer une partie de la criticité. De plus, quand la donnée du rapport d'approvisionnement évolue, les formules de calcul de ces deux critères n'ont pas besoin de changer. Les paramètres d'impacts sont les éléments les plus détaillés qui influencent la criticité.

Comme indiqué précédemment, la méthodologie inclut le modèle d'évaluation. Pour faciliter la compréhension et démontrer cette méthodologie, le modèle d'évaluation sur un cas basique est développé. Le cas basique est le cas où les paramètres sélectionnés sont possibles à évaluer et importants en général et où il n'y a pas de préférence. Pour ce modèle, une et

parfois plusieurs méthodes de calculs sont proposées pour certains critères. Les relations entre les paramètres d'impact et les critères du scénario basique sont déterminées (figure 20). En général, le modèle est une possibilité d'expression de la méthodologie. Ce modèle basique implique 21 paramètres d'impact. La criticité est représentée par 11 critères. Les formules sont précisées dans le chapitre 5.

Concernant présentation de la criticité, les résultats de ces 11 critères sont arrangés dans un bon ordre en premier. Le bon ordre veut dire que quand la valeur augmente, il contribue plus à la criticité. Puis nous prenons leurs valeurs relatives. Finalement, toutes ces valeurs sont devenues positives ou dans une même échelle avec la fonction exponentielle ou arc tangent. Avec ces traitements, les valeurs des différents critères peuvent être comparées et leurs seuils vont tous devenir identique (1). La somme de ces critères représente la valeur générale de la criticité. La criticité peut aussi être présentée par l'histogramme et la carte radar qui inclut la valeur de chaque critère. L'automatisation des mesures d'atténuation n'est pas encore réalisée dans ce modèle basique, c'est un travail qui reste en perspective.



Figure 20 : Connections entre des paramètres d'impact (rectangles blancs) et des critères (rectangles bleus) dans le scenario basique

L'étude de l'intégralité peut être réalisée par le taux de couverture des paramètres d'impact. Comme indiqué dans la partie diagnostic, un diagramme qui contient le groupe des paramètres d'impact est généré. Cependant, ils ne peuvent pas être tous couverts dans chaque étude en raison de la limitation de mains d'œuvre, du temps, du budget, etc. Tous les paramètres ne sont pas possibles ou faciles à évaluer en ce moment pour certaines entreprises. Théoriquement, une étude qui contient tous ces paramètres est plus complète et ses résultats sont aussi plus fiables. Le taux de couverture des paramètres représente donc l'intégralité et la fiabilité de l'étude dans un certain degré.

Comme le traitement final des résultats des critères rend la criticité d'une valeur relative, le fait de changer un input de tous ces matériaux n'influence pas la criticité à la fin. L'étude de sensibilité peut être réalisée en modifiant seulement un input d'un matériau individuellement.

#### Validation

Concernant la validation de la partie diagnostic, l'étude de cas intégrale sur les terres rares sert à compléter et améliorer cette partie. Cette étude sert aussi de vérification du mécanisme de la criticité. Après que le noyau de recherche (la partie diagnostic) soit établi, la méthodologie et le modèle d'évaluation quantitatif ont été proposés précédemment. Afin de vérifier leur faisabilité, deux applications ont été réalisées. Une première concerne les aimants et la deuxième les diodes lumineuses. Il est important de souligner que les criticités obtenues par le modèle d'évaluation dans le cadre de ces applications sont des résultats spécifiques au scénario, elles ne sont pas directement applicables à d'autres cas concernant les mêmes produits. C'est pourquoi dans cette partie, l'accent a été mis sur le processus et la démonstration du principe plutôt que de présenter les scores obtenus. Par ailleurs, les difficultés liées à l'accès aux données rencontrées lors de l'étude de ces applications ne seraient pas un problème lors de l'application de ce modèle par une entreprise qui veut analyser ses propres produits.

Pour l'application sur les aimants, deux matériaux sont analysés : le néodyme (un élément de la famille des terres rares) et le fer. L'utilisateur de ce modèle est une entreprise fictive – Magnet Expert Co. qui produit des aimants permanents et est située en France. Elle veut analyser la criticité des matériaux présents dans leur produit nommé le « Super magnet » qui a

pour formule chimique Nd-Fe-B. Les teneurs de ces trois matériaux sont de 36% pour le néodyme, de 63% pour l'acier et de 1% pour le bore (刘光华, 2007). Je suppose que la production planifiée du « Super magnet » est de 100 tonnes et qu'il y a 10% de perte de matériaux pendant la production. Pour récolter ces données, cinq profils sont établis. Le premier profil rassemble les données directement liées aux matériaux: les noms des matériaux, leurs codes (Mi), leurs pourcentages de masse dans le produit, la quantité demandée (dérivée de la suggestion précédente), le montant de réserve mondiale, le montant de production mondiale, la toxicité humaine et le taux de recyclage (données réelles). Le deuxième profil regroupe les informations techniques. Les candidats des substitutions du néodyme (Nd) sont le praséodyme (Pr), du samarium (Sm) et un mélange des terres rares. Les candidats des substitutions du fer (Fe) sont le cobalt (Co), le magnésium (Mg), le chrome (Cr) et le nickel (Ni). Une structure des fonctionnalités est établie selon l'interprétation de l'auteur sur les fonctions de l'aimant permanent. Le produit contient trois fonctionnalités générales: propriétés physiques, propriétés thermales et propriétés magnétiques. Ces trois groupes sont ensuite divisés en 13 fonctionnalités: le support physique, la dureté, la densité, la température de service maximum, la température Curie, l'énergie magnétique maximum (BH) max, l'induction résiduel (Br), la densité du flux magnétique résiduel et la coercivité. L'importance de chacune de ces fonctionnalités est notée selon l'interprétation de l'auteur. Une partie des valeurs de ces fonctionnalités (indicateurs) sont des données réelles qui viennent d'autres études publiées. Une autre partie est dérivée des données réelles. Le troisième profil assemble les informations liées à l'approvisionnement. Six fournisseurs sont imaginés dont quatre satisfaisant déjà la demande et deux autres étant des sources alternatives disponibles pour l'approvisionnement. Les informations de ces fournisseurs (comme la location et le prix) sont dérivées d'entreprises réelles qui sont trouvées sur internet. Les pourcentages d'approvisionnement sont décidés de façon aléatoire. Les noms des fournisseurs et leur capacité d'approvisionnement sont aussi fictifs. Le quatrième profil regroupe les données liées à la géographie. En fonction du profil d'approvisionnement, les informations de location des fournisseurs sont extraites en premier. Ensuite les pourcentages d'approvisionnement basés sur les pays sont extraits. Les données de stabilités des pays et sur les accords d'échanges économiques bilatéraux entre le pays d'achat et les pays d'approvisionnement sont aussi collectées. Le dernier profil concerne l'aspect législatif. Les restrictions potentielles venant de l'aspect législatif sont analysées. Suite à la collecte de données grâce à ces profils,

11 critères sont utilisés pour calculer la criticité des matériaux. Les détails des formules et des exemples de calculs sont illustrés.

Pour la présentation des résultats, un tableau contenant la procédure du traitement des résultats est présenté, suivi par les scores généraux de la criticité et une carte radar qui contient les notes de chaque critère du néodyme et du fer. Une étude de l'intégralité a été réalisée à la fin.

Comparée à l'application précédente, celle sur la diode luminescente est plus complexe. Premièrement, le produit contient plus de pièces (et matériaux) et sa structure est plus complexe. Elle permet de montrer comment traiter différemment les produis simples et ceux qui sont plus compliqués. Deuxièmement, cette application contient plus de données réelles. Troisièmement, une application supplémentaire permet de mieux démontrer la méthodologie et le modèle d'évaluation.

Dans la deuxième application, les informations de la diode luminescente sont basées sur celles de la lampe Philips Endurant LED. Le site de production est situé en France. La demande du produit égale à la valeur arrondie de la part de marché de la lampe Philips. Les 12 matériaux analysés sont les suivantes : Ce <sup>3+</sup>:YAG, TMGa, TMIn, TMAI, Al, Ni, Ag, Ti, W, Alumina, AuSn et Au. Comme la première application, les données de celle-ci sont aussi collectées sous des différents profils. Pour le profil lié aux matériaux, une approche différenciée que l'aimant a été utilisée. Comme une partie des matériaux analysés contiennent plus d'un élément, certaines données sont dérivées de leurs éléments individuels. Par exemple, la réserve globale de l'AuSn est un résultat dérivé du rapport de masse des éléments et de leurs réserves minérales correspondantes. Plus de détails sur des différents niveaux des matériaux sont présentés dans la figure 26.



Figure 26: Stratification des données de consommation de matériaux pour la production de LED dans cette application

Pour le profil technique, le produit est analysé sous 7 fonctionnalités générales divisées en 15 fonctionnalités. L'importance des fonctionnalités et des valeurs fonctionnelles est déterminée par le résultat des sondages conduits auprès de quatre experts. Un mélange entre la méthode Delphi et le Processus Analytique Hiérarchique est appliquée pour traiter les données. Pour le profil d'approvisionnement, trois fournisseurs par matériaux sont choisis au hasard parmi des entreprises réelles capables de fournir les matériaux. Les données (le prix, la capacité de production, leurs locations, etc.) sont issues de leurs pages internet de vente ou de communications directes avec l'entreprise. Comme certaines entreprises peuvent fournir plusieurs matériaux, un total de 24 entreprises est sélectionné comme fournisseurs. Le profil géographique contient 6 pays d'approvisionnement et le pays d'achat. Il a été traité de la même façon que dans la première application. Comme l'aspect législatif ne présente pas du danger, il n'est pas inclut dans cette application. La limite de temps et de données fait que certains critères ne sont pas analysés. À la fin, 8 critères sont analysés : « le déséquilibre entre la demande et l'approvisionnement », « la valeur », « le degré d'impact environnemental », « la qualité de la relation avec les fournisseurs », « l'épuisement de réserve », « la géo-relation
entre le pays d'achat et le pays d'approvisionnement », « la stabilité et la facilité de commercer avec les pays d'approvisionnement » et « le taux de recyclage ».

Les résultats du modèle contiennent un histogramme qui montre les scores généraux des criticités des matériaux (figure 30) et des cartes radars (figure 31). Comme le nombre de matériaux est plus grand, les matériaux sont présentés sous trois groupes pour faciliter la présentation et le classement des matériaux dans différents niveaux. Une autre différence de cette application est que les seuils critiques dans chaque critère sont déterminés à 20% au lieu d'être prédéterminés comme dans la première application. Le modèle d'évaluation laisse l'utilisateur choisir les seuils, ce qui nous permet de voir l'influence de ces seuils sur les résultats obtenus. Les détails des sources des données ainsi que les résultats générés pour différents seuils ou ajustés par la fonction exponentielle sont présentés dans les annexes.



Figure 30: Résultats généraux de la criticité des matériaux de LED avec les contributions des scores de chaque critère: 20% critique (seuil), ajusté par la fonction arc-tan



Figure 31: Cartes radars de la criticité des matériaux du LED divisés en trois groupes

Concernant l'étude de sensibilité, 12 inputs sont extraits tant que variables et sont groupés dans la vecteur x. 9 outputs sont observés et groupés dans le vecteur y. Par la suite, deux approches sont utilisées. La première est d'observer comment les résultats de la criticité changent quand les inputs de tous les matériaux sont augmentés de 10% ou de 100% de manière simultanée. Le résultat confirme la prédiction que la criticité ne change pas quand les inputs non-zéro de tous les matériaux ont tous changé dans la même proportion de changement et quand le changement ne dépasse pas leurs intervalles respectifs. La deuxième approche est d'augmenter de 10% ou 100% un seul input pour un seul matériau à un moment donné. Cette approche est plus proche des situations réelles. Pour conclure, 1) les paramètres (inputs) impactent différemment la criticité en termes de degré d'influence (de façon négative

ou positive). 2) un même input a peut-être une influence différente en fonction des différents matériaux. De plus, une étude de l'intégralité a été conduite comme dans l'application sur l'aimant. Parmi 39 paramètres d'impact, 22 sont sélectionnés dans le cas basique dont 77% sont couvert dans l'application de la diode luminescente.

## **Discussion et Perspectives**

#### Simplicité et Exhaustivité

D'un côté, le fait de simplifier les méthodes de calculs ou de diminuer le nombre de paramètres d'impact réduit la quantité des données exigées ainsi que le temps nécessaire pour réaliser l'évaluation. D'un autre côté, l'augmentation des données et de paramètres d'impact améliore la précision du résultat. Un compromis entre la simplicité et l'exhaustivité est nécessaire quand nous appliquons la méthodologie.

## Le fil de la pensée et l'ordre de mise en place de la recherche de la criticité

Le fait que la majorité des études sur les matériaux critiques soit apparues juste après la crise des terres rares en 2010, peu de temps s'est écoulé pour permettre de valider les résultats. C'est peut-être pourquoi les études commencent directement par développer une méthodologie d'évaluation afin de désigner des matériaux critiques dans leur périmètre de recherche. Cependant, l'ordre logique pour exécuter une étude sur la criticité est d'analyser ce qu'est la criticité (première phase), puis développer la méthodologie d'évaluation (phase intermédiaire) et finalement de chercher des solutions (phase finale). Sans la première phase, nous ne pouvons pas justifier la qualité des résultats produits par la phase intermédiaire.

### L'usage potentiel de la méthode d'Analyse du Flux des Matériaux (MFA)

Pendant l'application de la méthodologie sur les deux produits, je trouve que la MFA nous permettrait de présenter une carte générale et les chiffres exacts du flux de chaque matériau. Elle peut aussi nous fournir certaines données pour les calculs, ainsi que des supports pour trouver de meilleures approches d'atténuation.

## Les obstacles et les difficultés rencontrés lors d'une étude sur la criticité

Premièrement, la complexité des produits a rendu difficile la détermination des matériaux contenus. La sous-traitance et la confidentialité industrielle ont aussi augmenté la difficulté de remonter jusqu'aux matières première et d'obtenir des données tout au long de la chaine

d'approvisionnement. Deuxièmement, une étude complète sur la criticité concerne plusieurs départements de l'entreprise et même des intervenants extérieurs. Ceci représente du temps et a un coût. Troisièmement, la collecte et la quantité de données sont des problèmes majeurs. Le manque de données ou des données de mauvaise qualité diminuent la fiabilité du résultat. Quatrièmement, les changements de situations, y compris l'évolution des technologies, des marchés, etc., augmentent la difficulté d'établir de manière exacte des scénarios et mettent plus de pression sur le temps de réaction des acteurs. De plus, le phénomène des matières critiques lui-même force les acteurs concernés ou non concernés à réagir. Les mesures d'atténuation prises par différents acteurs modifient aussi la situation.

#### Indicateurs et méthodes de calculs

Certains indicateurs ou méthodes de calculs sont développés pour cette thèse. En l'état actuel de mes connaissances personnelles, les indicateurs sont discutables et une future amélioration de ceux-ci est possible. Par ailleurs, la pertinence des indicateurs ne sont pas prouvés dans cette thèse. Néanmoins, la pertinence des indicateurs dans les autres méthodologies développées dans le passé n'a pas été prouvée non plus, y compris celles développées par la Commission Européen ou le Département de l'Énergie. C'est pourquoi la méthodologie et le modèle d'évaluations proposés dans cette thèse sont davantage une suggestion ou un guide général destiné aux personnes souhaitant réaliser une étude de la criticité plutôt qu'une solution unique à tous les problèmes de criticité.

#### Pondération et subjectivité

Au début de ma thèse, je voulais minimiser ou même éliminer la subjectivité de la méthodologie d'évaluation. Cette idée s'est avérée difficile voir naïve après avoir fini de modéliser la méthodologie. Nous ne pouvons pas éviter la subjectivité dans les parties suivantes : les pondérations (des importances et des valeurs des fonctionnalités, du poids des critères etc.) et même l'établissement du scénario (la portée, la liste des matériaux à analyser, la détermination des fonctionnalités etc.).

## Réglage du seuil

Dans la méthodologie, deux moments exigent un réglage du seuil : l'évaluation de substituabilité et la normalisation des critères. Le seuil dans l'évaluation de substituabilité est lié aux cahiers des charges. Il est lié aux demandes des clients, des normes de conceptions ou

de production et des cibles de l'entreprise. Il peut donc être déterminé par des experts techniques et aux exigences précédentes. Pour le seuil des critères, j'ai proposé deux moyens. Le premier est d'utiliser un rapport fixe (comme 20% ou 30% est considéré critique) qui représente le pourcentage des matériaux que l'entreprise veut mettre en priorité. Un autre moyen est de laisser déterminer le seuil exact de chaque critère.

#### L'usage potentiel de la méthodologie proposé

Premièrement, il est possible d'adapter cette méthodologie au niveau d'un secteur avec certaines modifications (de la portée, de certains indicateurs, des données), c'est-à-dire évaluer les criticités des matériaux au niveau du secteur du produit de manière générale au lieu d'étudier une entreprise spécifique. Deuxièmement, il est possible d'utiliser la méthodologie afin d'évaluer les criticités des composants qui contiennent plusieurs matériaux au lieu d'un métal ou d'une matière première.

#### Limitations et points à améliorer

Les deux applications manquent de coopérations industrielles. Les entreprises qui produisent l'aimant et la diode luminescente et certaines informations des fournisseurs sont imaginées. Même si la deuxième étude contient plus d'informations réelles, ses résultats ne peuvent pas être utilisés directement par les autres entreprises. De plus, l'aspect subjectif de l'étude et la limite de mes connaissances personnelles ont rendu certaines données moins fiables. Cependant, ces limitations peuvent être minimisées dans le cas d'une application concrète par une entreprise réelle ou des experts. La méthodologie est censée convenir à tout type de matériaux, mais ces deux applications analysent seulement des métaux.

Concernant les points à améliorer, trouver des poids appropriés des critères peut permettre d'augmenter l'exactitude du résultat de l'étude de la criticité. Compléter la base de données des approches d'atténuation et les intégrer dans le modèle d'évaluation permet aussi de rendre les résultats plus complets. Une justification des indicateurs et une application de la méthodologie pour un cas réel historique pourrait aider à vérifier la pertinence de la méthodologie. Par ailleurs, il est aussi possible de remplacer certaines méthodes de calculs dans le futur si nous trouvons de meilleurs choix.

## Conclusion

Les questions de recherches et les réponses

Cette thèse est guidée par les questions de recherches suivantes :

- 4 Qu'est ce qui a déjà été fait dans le domaine de la recherche de criticité ?
- 4 Comment définir la criticité des matériaux (au niveau du produit)?
- 4 Comment déterminer la criticité des matériaux (au niveau du produit) ?

La première question de recherche a trouvé réponse dans le chapitre « État de l'art » qui a servi de ligne directrice pour la suite des travaux de recherche. Dans l'ensemble, le phénomène des matières critiques est déjà apparu longtemps dans le passé. Cependant, ce genre de phénomène nommé « critique » marque une séparation avec d'autres termes similaires tels que « stratégique », « disponible », « rare » etc. Le plus ancien document officiel parmi des études examinées qui mentionne le terme « critique » est un mémorandum américain « Des matières premières importées critiques » publié en 1974. 34 ans plus tard, le Conseil National de Recherche des Etats-Unis a développé une matrice de criticité pour évaluer la criticité des matières premières et cette matrice a servi comme concept de base pour deux études réputées : celle de la Commission Européenne et celle du Département de l'Energie en 2010. C'est donc en 2008 que la recherche sur la criticité a débuté et en 2010 que ce terme est devenu connu grâce à la crise des terres rares et à ces deux études. Jusqu'à présent, il existe des études sur des matières prédéterminées critiques et sur des matières dont la criticité est déterminée à l'aide d'une méthodologie d'évaluation. Parmi les études basées sur une méthodologie, certaines ont une portée régionale comme par exemple l'étude qui analyse les matières critiques pour l'Union Européenne. Certaines études sont conduites à l'échelle ont une portée de la technologie comme par exemple, l'étude du Département de l'Energie qui analyse les matières critiques pour l'économie d'énergie propre. Certaines études analysent la criticité d'un groupe de matériaux spécifiques, par exemple, l'Université de Yale qui a analysé la criticité des métaux du groupe cuivreux, etc. Par ailleurs, il existe aussi des études qui s'intéressent aux impacts des matières désignées critiques par les études précédentes sur leur pays ou qui s'intéressent aux approches d'atténuation pour ces matières critiques. Dans toutes les études examinées, la majorité viennent soit d'Europe soit des Etats-Unis (qui sont plus sensibles à la production de hautes technologies ou à l'importation des

matières premières pour les hautes technologies). La majorité des organisations qui ont conduit une étude de criticité répondent directement à un besoin gouvernementale ou ont un lien proche avec le gouvernement.

Cet état de l'art m'a permis de déterminer trois lacunes de recherches. Premièrement, il n'existe pas d'étude compréhensive qui diagnostique la criticité : quel est le mécanisme de la criticité, quels éléments influencent la criticité et comment l'influencent-elles. Deuxièmement, parmi toutes les méthodologies d'évaluation, il n'en existe pas au niveau du produit. Ceci permet à l'entreprise de connaitre la criticité des matériaux de leurs propres produits. Troisièmement, les liens entre le mécanisme de la criticité, les méthodologies d'évaluation et les propositions d'approches d'atténuation ne sont pas établis.

Pour la deuxième question de recherche, voici la définition proposée : La criticité d'un matériau est une valeur relative à l'interaction entre l'importance de la matière pour le sujet, le déséquilibre entre la demande et l'approvisionnement, et l'accessibilité à cette matière. La criticité est renforcée par les changements brusques ou les situations où les acteurs ne sont pas en mesure de s'adapter.

Toutes les matières sont importantes dans un certain degré. Le mot « relative » implique que je n'ai pas ignoré l'importance des autres matériaux, mais souligné ceux qui méritent plus d'attention dans la situation spécifique. Le mot « sujet » implique que la criticité varie en fonction du sujet : analysons-nous la criticité des matériaux pour un pays, un type de technologie, un produit ? Quel pays, quelle technologie, quel genre de produit ? Le « sujet » et « l'acteur » permettent une interprétation dynamique ce qui permet d'adapter la définition à différentes situations. La dernière partie de la définition contient les informations suivantes: Aucun matériau ne peut être critique indéfiniment ; Un faible temps de réaction pour l'acteur aggrave la criticité ; La capacité d'adaptation à la nouvelle situation est un enjeu important pour déterminer la criticité des matériaux. L'étude de cas sur les terres rares justifie les arguments précédents.

Pour la troisième question de recherche, une méthodologie d'évaluation et un modèle d'évaluation quantitatif de la criticité des matériaux au niveau du produit sont développés. Les étapes principales de la méthodologie sont : Choisir le produit cible ; Choisir la liste des matériaux à analyser ; Établir le scénario ; Construire le modèle de calcul ; Sélectionner

l'indicateur approprié pour certains paramètres d'impact (optionnel) ; Entrer les données dans le modèle de calcul ; Analyser les résultats en fonction des outputs du modèle. Le modèle est une façon d'interpréter la méthodologie. Le modèle proposé est basé sur un scénario basique où des paramètres d'impact (jugés importants et quantifiables à un instant donné) sont sélectionnés et où il n'y a pas de préférence entre les critères. Ce modèle contient 11 critères pour déterminer la criticité et génère deux types d'outputs, des scores généraux de la criticité et des cartes radars qui montrent ce qui contribue à la criticité. La démarche pour effectuer l'étude d'intégralité et de sensibilité est aussi présentée. Finalement, le modèle d'évaluation a été appliqué à deux produits: l'aimant permanent et la diode luminescente. Ces applications m'ont permis d'améliorer, de démontrer et de justifier la faisabilité du modèle développé.

## Liste de contribution de cette thèse

La liste des contributions est ci-dessous:

- Une carte générale du domaine de la recherche sur la criticité.
- Un diagnostic compréhensif sur le mécanisme de la criticité.
- Une nouvelle définition de la criticité.
- Une méthodologie d'évaluation au niveau du produit avec une illustration à l'aide d'un modèle d'évaluation quantitatif pour un cas basique.
- Des méthodes de calculs des critères proposés dans le modèle
- Des propositions pour traiter des données dans le modèle
- Une nouvelle approche pour intégrer l'aspect dynamique dans l'évaluation de la criticité

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## Développement d'une méthodologie d'évaluation de la criticité des matériaux au niveau du produit

Les impacts causés par la crise des terres rares en 2010 mettent en évidence l'importance des matériaux et ont conduit en un intérêt accru dans la recherche sur leur criticité. Cette thèse s'ouvre par un état de l'art qui présente et évalue les travaux existants dans ce domaine et met en évidence trois lacunes de la recherche sur la criticité des matériaux (l'absence d'un véritable diagnostic de criticité; l'absence d'une méthodologie d'évaluation de la criticité au niveau produit; le défaut de lien bien établi entre mécanisme de criticité, méthode d'évaluation et solutions proposées). En consé-quence, la thèse comble les deux premières lacunes et offre plusieurs pistes à l'égard de la troisième. Concernant le diagnostic de la criticité d'un matériau, la thèse propose d'illustrer le mécanisme de criticité par quatre dimensions : le déséquilibre entre offre et demande ; l'importance du matériau pour le produit l'accessibilité de l'approvisionnement ; et les facteurs dynamiques. Une définition de la criticité est proposée. Le mécanisme de criticité étant au centre de la recherche, une méthodologie permettant de déterminer la criticité matérielle à l'échelle « produit » est développée et complétée par un modèle applicatif quantitatif. La méthodologie offre un raisonnement général pour conduire une étude de la criticité ; le modèle illustre une de ses possibilités d'être appliqué à des cas réels pour déterminer quantitativement la criticité. A la fin, l'application du modèle à deux produits (l'aimant permanent et la diode électroluminescente) est présentée.

Mots clés : développement durable - prise de décision - planification stratégique - matériaux - produits industriels.

Development of Materials Criticality Profiling Methodology at Product Level

Rare earth crisis in 2010 showed the importance of some materials and whipped up interest in the research on material criticality. A review work was first conducted in order to get a better understanding of the existing work in this research area and to see where more work is needed. Based on this review, three research gaps were identified (lack of a comprehensive diagnosis of criticality; lack of evaluation methodology at the product level; lack of links between the mechanism of criticality, the evaluation methodology and the solutions offered. This thesis focuses on the two first research gaps and offers several ideas for the last one. Regarding diagnosis of criticality, the mechanism is illustrated under four dimensions: imbalance between supply and demand, importance of the material to product, supply accessibility and dynamic factors. A definition of criticality is also put forward. Considering the established mechanism as research core, a methodology to evaluate the criticality of materials at the product level has been developed and is completed with a concrete and quantitative model. The methodology offers guidance on how to assess criticality and sets a framework for evaluation. The model illustrates a way to use this methodology through a tool that assigns a 'criticality score' to materials and shows how the score is contributed. The calculations were automated in Excel. Two applications, one for permanent magnet and the other for light emitting diode, were conducted to demonstrate and improve the methodology and the model.

Keywords: sustainable development - decision making - strategic planning - materials manufactures.

Thèse réalisée en partenariat entre :





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