Towards a dynamic criticality assessment: Linking agentbased demand - with material flow supply modelling approaches

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Abstract:

Emerging technologies such as information and communication-, photovoltaic- or battery technologies are expected to significantly increase the demand for scarce metals in the near future. The recently developed methods to evaluate the criticality of mineral raw materials typically provide a 'snapshot' of the criticality of a certain material at one point in time by using static indicators both for supply risk and for the impacts of supply restrictions or economic importance. While allowing for insights into the mechanisms behind the criticality of raw materials, these methods cannot account for continuous changes in products and/or activities over time. We propose an approach which goes beyond this static state of the art insofar as it includes the dynamic interactions between different possible demand and supply configurations as a precondition for the evaluation of criticality. The framework developed integrates an agent-based behavior model, where demand emerges from individual agent decisions and interaction, into a dynamic material flow model, representing the materials' stocks and flows across their lifetime. Within this framework, the evaluation of criticality is exemplarily specified for the environmental dimension by applying life-cycle assessment methodology.

Keywords: Integrative modeling, material flow analysis, agent-based modeling, criticality assessment, scarce metals, life-cycle assessment.

1. Introduction

Emerging technologies such as information and communication-, photovoltaic- or battery technologies are expecting to significantly increase the demand for scarce technology metals in the near future (Angerer et al. 2009; Waeger et al. 2010; Weil et al. 2009). Recently, concern over disruptions to raw materials supplies has risen as a consequence of China's rare earth commodity export restrictions to 30,258 metric tons in 2010 (Yu 2010). Today, China controls 97% of the supply to the world market for rare earth commodities (Figure 1) (Corfield 2010; Du and Graedel 2011). This confronts high-tech industries with a 40% reduction in available raw materials of that group of elements, demonstrating the vulnerability of the high-tech EU economy in times of acute supply disruption (Kooroshy et al. 2010). For the ICT-, aerospace-, automotive- and electronics industries, there is a risk that supply disruptions will constrain technological progress in the near future, which is why rare earth and platinum group metals are often referred to as "critical" materials (EC 2010; NRC 2008). In this content the European Commission has raised the issue of supply risks related to critical materials in general and rare earth metals (REM's)¹ and platinum group metals (PGM's)² in particular (EC 2010).



Figure 1: Global production of rare earth oxides 1950-2007 (Picture taken from Du and Graedel (2011)).

Measuring materials' criticality only by the relative abundance of chemical elements in the Earth's upper continental crust might be misleading. In this regard, the relatively wide-spread REM's, for example, do not belong to the most scarce metals (USGS 2002). Ra-ther, as shown by e.g. China' supply dominance of the last years (Du and Graedel 2011) and its ability to control its exports (Yu 2010), materials criticality is a multifactorial issue (see e.g. (NRC 2008); (Waeger et al. 2010)).

¹ Rare Earths is a group of 17 chemical elements: scandium (Sc), yttrium (Y) and the 15 lanthanides (La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu).

² The platinum group metals consist of ruthenium (Ru), rhodium (Rh), palladium (Pd), osmium (Os), iridium (Ir) and platinum (Pt).

Recently, several static indicator-based criticality assessment methodologies have been developed, for example by the US National Research Council (NRC) (NRC 2008) and the EU (EC 2010). Both methodologies condense the various criticality aspects into two dimensions of a criticality matrix, the supply risk (US: risk of supply restriction) on one axis and the economic importance (US: impact of supply restriction) on the other. A material is labeled "critical" when the risks of supply shortage and their impacts on the economy are higher than for most of the other raw materials. While the EU study analyzes the criticality of 41 raw materials across all industrial sectors (EC 2010), the US study concentrates on eleven elements or element groups, respectively, relevant for the US economy (NRC 2008). While the NRC study evaluates criticality based on the judgment of the committee, the EU study developed a quantitative approach. In the EU study the economic importance is measured by a breakdown of the value added attributed to a raw material and the supply risk by the production of raw materials (i.e. the level of the worldwide production linked with the political and economic stability of the producing countries), the substitution potential (i.e. substitutability index) and the recyclability (i.e. recycled content) (EC 2010). The NRC considers the fragility if the existing market, production concentration, reliance on byproduct sources of supply, opportunities of developing alternative sources to evaluate the importance of a supply restriction. The supply risk is evaluated by considering geological, technical, environmental and social, political, and economic availability (NRC 2008). The application of these methodologies resulted in fourteen raw materials to be considered as critical in a European context, and five to be considered critical in a United States context. In both studies REM's and PGM's were identified to be critical.

By using static indicators, a 'snapshot' of the criticality of a certain material at one point in time is provided; changes in products or activities over time are not accounted for. Furthermore, feedbacks between possible demand - and the supply chain developments, and their effects on the background systems on which these products and activities depend (e.g. the supply of electricity) are not explicitly considered. Two basic assumptions on which such an approach is typically based upon are (i) that a single substitution decision (demand) does only marginally affect the supply chain, and (ii) that the criticality of certain materials stays constant over time.

(i) Material substitution decisions of large international companies might induce changes in the supply chain (e.g. the installation of new mining facilities) and therefore affect the materials' criticality. To take such decisions based on a static criticality assessment might be misleading. In addition, the induced production capacities will occur with a certain time delay and therefore will be accompanied by a short term supply restriction. Furthermore, even if the companies' substitution decisions do not significantly affect the supply chain, materials criticality might dramatically change due to an increasing demand from other sectors (e.g. an increased Indium price for thin-film photovoltaic driven by the demand for flat screens) or geopolitical constraints (e.g. China's REM's export limitation or production dominance (Yu 2010)). (ii) First approaches to consider criticality with dynamic models have been reported for PGMs (Alonso et al. 2008). Recently, Du and Graedel (2011) quantified the stocks and flows of REM from 1995 - 2007. However, none of the approaches included the interrelation of individual industrial decisions and supply-chain development.

Furthermore, in order to better anticipate the environmental challenges related to their mining and manufacturing, analytical progress in life cycle assessment of REM's and PGM's is required (Althaus and Classen 2005; Du and Graedel 2011; EC 2010). That is, new approaches are needed not only to include the interactions of demand and supply parameters of REM's and PGM's, but also to address their dynamic changes over time and related environmental impacts along the materials life cycle.

2. Conceptual framework

Our approach aims at advancing criticality assessment by dynamically modeling the factors affecting criticality partly outlined above, and by assessing the related environmental risks from a life cycle perspective. It is designed to investigate how far criticality will be affected by industrial substitution decisions if dynamic interrelations are intended to be considered.

Figure 2 shows the conceptual framework for coupling a dynamic behavior with a dynamic material flow model to simulate the (economic and ecological) consequences of materials substitution decisions under constraints (i.e. different scenarios). Simulation experiments with the coupled models result in the material availability at a certain point in time, to a certain price and to a certain environmental impact. In addition, the simulation experiments allow for assessing the probabilities of these material availabilities for a particular scenario. This is, the coupled dynamic model provides the basis for assessing the environmental risks (i.e. probability of certain outcome) related to material substitution decisions.

The dynamic material flow model aims at simulating the material flows across their life cycle. For this purpose, all relevant production and recycling routes (processes and flows) have to be analyzed and modeled. Because metal ores do usually not contain single elements but a range of different elements, which is particularly true for REM's and PGM's, the dependencies with other main and by products have to be analyzed. In addition, the environmental impacts along the production chain of REM's and PGM's are considered and modeled depending on ore quality and on the materials technical performance and durability. This allows for understanding the interdependencies between environmental impacts and inter alia, demand and product/ by-product ratios. Furthermore, it allows showing if recycling is feasible and how relevant its contribution can be for supply security. The material flow model builds the frame (i.e. the technical environment) for the dynamic behavioral model.

The dynamic behavior model aims at understanding and simulating the dynamic interrelation between the substitution decisions and the underlying material flow system. For this purpose, it focuses on how substitution decisions affect each other and how they are interrelated with the material flows down-stream and upstream the consumption chain. The demand of REM's and PGM's is determined by the substitution decisions of different companies and their interaction. An agent-based modeling (ABM) approach allows for modeling these interacting actors in view of assessing how they cumulatively affect the material flow system. Agents, their behavior and their environment are the three basic components of an agent based model. Agents are the representatives of real world actors (e.g. companies) within the model. This approach requires the identification of those agents that demand for REM's and PGM's, as well as an analysis of the interactions among agents, and the agent specific decision-making (intention) and behavior (Knoeri et al. 2011). The material flow and agent-based models allows for understanding how the interacting agents affect the material flows under which condition (i.e. framework scenarios).



Figure 2: Conceptual framework for the dynamic material flow and behavior model (blue boxes stand for processes, solid blue arrows for the flows in the material flow model; green boxes indicate the substitution decision taken by the individual companies/industrial sectors, green-dotted arrows indicate the interrelation of these decisions among themselves and with their environment in the dynamic behavior model; the light brown box defines the scope of the environmental risk assessment assessing the resource inputs from and emissions to nature indicated by purple arrows)

Framework scenarios: A small set of consistent scenarios is key for assessing future development and case study research (Scholz and Tietje 2002; Tietje 2005). The important scenario parameters required for the material flow - and the behavior model should be derived from the respective conceptual models. A possible approach to assess the interrelations between the different parameters and to identify a consistent set of scenarios consists in performing a scenario workshop (Wiek 2002).

Environmental risk assessment: In general, 'risk' refers to the uncertainty about and the severity of the consequences (or outcomes) of an activity with respect to something that humans value (Aven and Renn 2009). In the context of materials' substitution, risk can be seen as the probabilities and extent of environmental consequences when substituting one material with another. Environmental consequences are the environmental impacts related to the life cycle of the products with different material substitutes. The probabilities of the consequences of a substitution decision are calculated from the coupled model. The severities of the environmental consequences are assessed with life cycle assessment (LCA).

3. Conclusion

The approach proposed to evaluate the criticality of raw materials goes beyond the current state of the art in the sense that it explicitly includes the dynamic interrelation between factors affecting criticality. Its application on two cases, REM's in Mg-alloys for high temperature applications and ceramic matrix compounds as substitutes for REM's for superalloys in gas turbines, is expected to provide the proof of concept for coupling a dynamic material flow and a dynamic behavior model for risk assessment. Our approach will enable to simulate dynamic market responses to substitution decisions as part of risk management strategy, to significantly advance the understanding of supply risk beyond the static indicator approaches currently proposed and enable a more systematic analyzes of complex market responses.

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