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Towards a dynamic assessment of raw materials criticality: Linking agent-based demand — With material flow supply modelling approaches

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HIGHLIGHTS

- ► Current criticality assessment methods provide a 'snapshot' at one point in time.
- ► They do not account for dynamic interactions between demand and supply.
- ► We propose a conceptual framework to overcomes these limitations.
- ► The framework integrates an agent-based behaviour model with a dynamic material flow model.
- ► The approach proposed makes a first step towards a dynamic criticality assessment.

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ABSTRACT

Emerging technologies such as information and communication-, photovoltaic- or battery technologies are expected to increase significantly 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. While allowing for insights into the mechanisms behind the criticality of raw materials, these methods cannot account for dynamic changes in products and/or activities over time. In this paper we propose a conceptual framework intended to overcome these limitations by including the dynamic interactions between different possible demand and supply configurations. The framework integrates an agent-based behaviour model, where demand emerges from individual agent decisions and interaction, into a dynamic material flow model, representing the materials' stocks and flows. Within the framework, the environmental implications of substitution decisions are evaluated by applying life-cycle assessment methodology. The approach makes a first step towards a dynamic criticality assessment and will enhance the understanding of industrial substitution decisions and environmental implications related to critical metals. We discuss the potential and limitation of such an approach in contrast to state-of-the-art methods and how it might lead to criticality assessments tailored to the specific circumstances of single industrial sectors or individual companies.

1. Introduction

Emerging technologies such as information and communication-, renewable energy generation-, and energy storage-technologies are expected to increase the demand for geochemically scarce metals[1] significantly in the near future (Angerer et al., 2009; Wäger et al., 2010, 2012; Weil et al., 2009). Recently, concern over disruptions to raw materials supplies has risen in the light of China's export restrictions – that controls 95% of the global supply of rare earth elements (REEs)[2] (Corfield, 2010; Du and Graedel, 2011) – causing the availability of these commodities to drop by 40% between 2009 and 2010 (from 50,149 to 30,258 metric tons) (Danlu, 2012; Yang, 2012; Yu, 2010). This demonstrates the vulnerability of high-tech industries in the 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. For this reason REEs and other geochemically scarce metals, such as platinum group metals (PGMs)[3] are often referred

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[1] A metal is considered as "geochemically scarce" when it occurs at an average concentration in the earth's crust below 0.01 wt.% (Skinner, 1979).

[2] The Rare Earth Elements (REEs) family includes 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).

[3] The Platinum Group Metals (PGMs) family consist of 6 elements: iridium (Ir), osmium (Os), palladium (Pd), platinum (Pt), ruthenium (Ru) and rhodium (Rh).

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to as "critical" raw materials (DOE, 2010; EC, 2010; NRC, 2008). In the following the issues related to critical raw materials are mainly illustrated with REEs and PGMs – since they provide some of the most evident examples – although the insights are generally transferable to most geochemically scarce metals.

Measuring raw materials' criticality only by the relative abundance of chemical elements in the Earth's upper continental crust can be considered as insufficient. In this regard, the relatively widespread REEs (USGS, 2002), for example, would not belong to the metals with the highest supply risk, as stated by the European Commission (EC) (2010). Rather, as shown by e.g. China's supply dominance of the last years (Du and Graedel, 2011) and its ability to control the exports (Yu, 2010), raw materials' criticality is a multifactorial issue depending on geological, geopolitical, technological, economic, ecological and social issues (see e.g. NRC, 2008; Wäger et al., 2010).

Recently, several static indicator-based criticality assessment methodologies have been developed, pioneered by the US National Research Council (NRC) (2008) and the European Union (EC, 2010). The US study laid the basis for the on-going criticality discussion by proposing the "criticality matrix" which condenses the various criticality aspects into two dimensions, the *supply risk or risk of a supply restriction* on one axis and the *impact of supply restriction or economic importance* on the other one. The *supply risk* is evaluated (i) on the short term by the fragility of the existing market, production concentration, reliance on by-product sources of supply, opportunities of developing alternative sources; and (ii) on the long term, by considering geological, technical, environmental and social, political, and economic availability. The *impact of a supply restriction* is evaluated by considering the difficulty of substituting a restricted material, where the consequences (i.e. economic costs) depend on the particular form of restriction (e.g. physical availability, technical and economic feasibility). A qualitative evaluation of criticality was accomplished by an expert committee, as in this pioneering study emphasis was given to evaluating the feasibility of the approach to measure criticality, concentrating on eleven elements or element groups, respectively, relevant for the US economy (NRC, 2008).

This criticality matrix approach was adopted by the EU study and extended with quantitative measurements. The *economic importance* is measured by a breakdown of the value added attributed to a raw material, and the *supply risk* by the concentration and stability of production of raw materials (i.e. the distribution 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. measured with the recycled content). The study analysed the criticality of 41 raw materials across all industrial sectors. A material was labelled as "critical" when the risks of supply shortage and their impacts on the economy are higher than for most of the other raw materials (EC, 2010).

The application of these methodologies resulted in fourteen raw materials that were considered as critical in a European context, and five considered critical in a United States context. According to a recent survey, the following elements or element families have most frequently been evaluated as critical in a selection of seven selected studies – including amongst others the two above mentioned and a study of the US Department of Energy specifically focusing on emerging clean energy technologies (DOE, 2010) – indium, niobium, platinum, REEs, rhodium, ruthenium and tungsten (Erdmann and Graedel, 2011).

Current static criticality assessment methods set the stage for the on-going criticality discussion across a wide range of elements. However, they exclude several interrelations relevant for criticality issues, partly as a consequence of their wide scope, but also because of limited data availability and the conceptual novelty of measuring criticality. Some important aspects that have not been fully accounted for so far include:

- changes in products or activities over time – by using static indicators, only a 'snapshot' of the criticality of a certain material at one point in time is provided – are not included[4];
- feedback between possible demand and 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. The presently applied "static" approaches implicitly assume that substitution decisions on the demand side only marginally affect the supply chain.

Previous studies recognize the potential dynamics affecting the criticality of elements but, owing to the complexity of these dynamics, limit their assessment to static analysis of a fixed time period. However, industrial stakeholders may still base their long-term decisions on those assessments and implicitly assume that criticality stays constant.

Thus dynamic criticality issues are often caused by interdependencies not included in previous assessments such as: 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 raw 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 in specific sectors do not significantly affect the supply chain, raw 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 REEs export limitation or production dominance Yu, 2010). First approaches to consider criticality with dynamic models have been reported for PGMs (Alonso et al., 2008) and REEs (Alonso et al., 2012). Recently, Du and Graedel (2011) quantified the stocks and flows of REEs from 1995 to 2007. However, none of the approaches included the interrelation of individual industrial decisions and supply-chain development and are therefore ill suited for industrial decision support.

In addition, environmental issues related to metals criticality have only been marginally considered in criticality studies so far, although metals' mining and manufacturing is known as having considerable environmental implications (Althaus and Classen, 2005; Classen et al., 2009). Graedel et al. (2012) have developed a methodology which extends the criticality matrix applied in the NRC study (NRC, 2008) by an environmental dimension based on available cradle to gate life cycle inventory data for the evaluated metals from the ecoinvent database (Hischier et al., 2010). Doing so, they separate supply restrictions due to regulatory measures, which is covered in the supply risk, from the environmental implications of utilizing particular metals, allowing for an independent assessment of environmental issues from other criticality aspect. As mentioned by Graedel et al. (2012) such accounting of environmental implications provides a snapshot in time, and environmental impacts might change with increasing demand that leads to the exploitation of lower ore grades and additional pressure on ecosystems. Furthermore, environmental impacts might appear with different probabilities and therefore have varying risk implications.

Hence, new approaches are needed not only to include the interactions of demand and supply parameters of critical raw materials, but also to address their dynamic changes over time and related environmental impacts along the materials life cycle. In this paper we present a conceptual framework that could be used to model the interrelated criticality aspects dynamically, elaborate on the potential and limitation of the approach, and discuss potential future research requirements.

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[4] This is why the ad hoc working group of the EC recommends updating the list of critical raw materials every 5 years (EC, 2010).

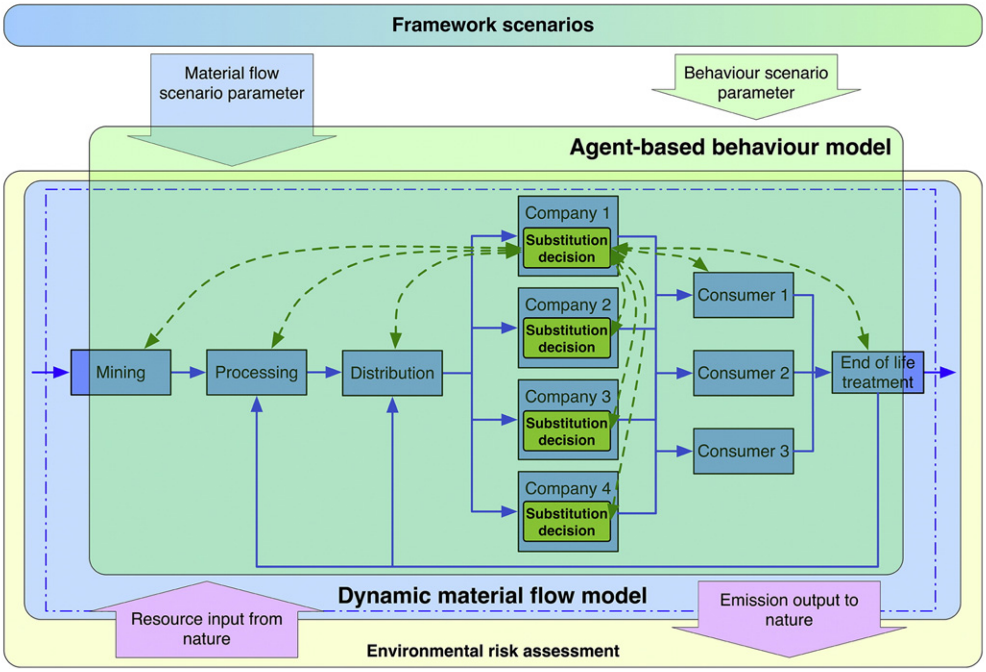

Fig. 1. Conceptual framework for the dynamic material flow and agent-based behaviour model (blue boxes stand for processes, solid blue arrows for the flows in the material flow model; green boxes indicate the substitution decision taken by the individual companies/industrial sectors, green-dotted arrows indicate the interrelation of these decisions among themselves and with their environment in the agent-based behaviour model; the light brown box defines the scope of the environmental risk assessment assessing the resource inputs from and emissions to nature, both indicated by purple arrows).

2. Conceptual framework

Our approach aims to advance existing criticality assessments by modelling the interrelated factors affecting criticality dynamically outlined in part 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 considered and thus might directly support such decisions.

The framework couples an agent-based behaviour model (describing the material substitution decisions of industries) with a dynamic material flow model (Fig. 1). This allows us to simulate the (economic and ecological) consequences of material substitution decisions under constraints (i.e. different framework scenarios). Simulation experiments will result in material availability distributions at a certain point in time, to a certain price and environmental impact. The coupled dynamic model therefore provides the basis for assessing the environmental risks (i.e. probability of certain outcomes) related to material substitution decisions. In the subsequent paragraphs the two models, framework scenarios, and the environmental risk assessment are addressed in more detail.

2.1. Agent-based model and dynamic material flow model

The dynamic material flow model aims to simulate the material flows across their life cycle. For this purpose, all relevant processes along a materials life cycle such as mining, processing, distribution, manufacturing within companies as well as usage and end of life treatment have to be analysed and modelled. Dynamic material flow analysis (MFA) has become a standard tool for forecasting material flows, assessing recycling schemes and related environmental impacts (e.g. Baccini and Brunner, 2012; Daigo et al., 2009; Hatayama et al., 2010; Muller, 2006).

Many scarce metals are not mined on their own but as by-products of other material mining, and therefore tied to the demand for the main metal (Graedel, 2011; Hagelüken and Meskers, 2010). Such interdependencies are evident for REEs and PGMs and define to a large extent which processes to include in the life cycle (i.e. system boundary definition). In addition, the environmental impacts along the production chain of REEs and PGMs are considered and modelled depending on ore grade and on the material technical performance and durability. This allows us to understand the interdependencies between environmental impacts and – inter alia – demand and product/by-product ratios. Furthermore, it reveals whether recycling is environmentally beneficial and how relevant its contribution can be for supply security. The material flow model builds the frame (i.e. the technical environment) for the agent-based behavioural model.

The agent-based behaviour model aims to understand and simulate 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 in the consumption chain. Today, such substitution decisions are taken to achieve marketing and engineering design goals which in turn are mainly based on consumer preferences and material properties with little account for the criticality of single elements (e.g. Krishnan and Ulrich, 2001). Once the product is established on the market, increased demand from other applications might restrict the availability of marginal elements such as REEs and PGMs. Such potential supply restriction can be seen as an emergent property of interacting agents across the supply–demand network, which can be captured with agent-based modelling (ABM) (Axelrod, 1997; Janssen, 2002; Tesfatsion and Judd, 2006).

ABM as a bottom-up approach is commonly used for analysing transition dynamics in socio-technical systems (Bergman et al., 2008; Chappin and Dijkema, 2010; Haxeltine et al., 2008). Its combination with top-down approaches such as global dynamic optimization or dynamic MFA allows for additional insights into e.g. what can be achieved with particular measures and what could create barriers to an implementation of such plans (Beck et al., 2008; Kempener et al., 2009). Until now, such a combination has mostly been applied to energy systems (Andrews et al., 2011; Axtell et al., 2001; Davis et al., 2010; Kempener et al., 2009). Just recently metal flows were explicitly addressed as Bollinger et al. (2012) contrasted MFA with an agent-based model including material entities (resulting in flows) for analysing different recycling schemes. They concluded that on the upside such an agent-based model allows for a more native representation of the societal material flow system, while on the downside the approach was more computationally intensive than top-down equation-based techniques.

The demand for REEs and PGMs is determined by the substitution decisions of different companies in different sectors, and by their interaction driven by the demand for the end product from the consumers. Agents, their behaviour and their environment are the three basic components of an agent-based model, with agents being the representatives of real world actors (e.g. companies) within the model. Hence, implementing such a model requires the identification of those agents that demand REEs and PGMs, as well as an analysis of the interactions among agents and the agent specific decision-making (intention) and behaviour (Knoeri et al., 2011). Depending on the focus of the study the main level of decision analysis might shift from industrial substitution decisions, as illustrated in Fig. 1, to consumer technology adoption. A combination of such an agent-based model with a material-flow model, which represents the agents' technical environment, allows for understanding how the interacting agents affect the material flows under which conditions (i.e. framework scenarios).

2.2. Framework scenarios

A small set of consistent *framework scenarios* is the key for assessing future development and case study research (Scholz and Tietje, 2002; Tietje, 2005). From the conceptual model the important scenario parameters required for the material flow, and the behaviour model, are derived. Some of these parameters might be consistent with criticality indicators and partly interrelated. Formative scenario analysis (Spoerri et al., 2009; Wiek, 2002) and cross-impact analysis (Weimer-Jehle, 2006) are possible approaches to assess such interrelations and to identify a consistent set of scenarios.

2.3. Environmental risk assessment

The framework concludes with an *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 can be assessed with life cycle assessment (LCA) (Frischknecht et al., 2007a,b,c).

3. Potential and limitations of the approach

The approach proposed aims to go beyond current criticality assessment based on static indicators by explicitly including the dynamic interrelation between industrial substitution decisions and the criticality of metals considered. By doing so, we expect to resolve some of the known shortcomings of existing approaches; however, this might result in other drawbacks. In the following we elaborate on the potential and limitations related to specific characteristics of the approach.

3.1. Dynamic vs. static

The proposed approach aims to assess the availability of scarce metals over time by explicitly modelling industrial decisions and their interaction and consequences on the materials' stock and flows. Such a dynamic assessment depends on the technology and decision knowledge available at the time of modelling. As a consequence, uncertainty about future technologies and in particular industrial decisions might limit the accuracy.

3.2. Explicit behaviour modelling

In contrast to current approaches, which implicitly anticipate actors' behaviour in their indicators, we propose to explicitly model actor behaviour. While this might be beneficial for the transparency of assumptions about industrial decisions it requires a thorough understanding of how substitution decisions are made and how they affect each other and the related supply stream actors. In turn it might greatly enhance the understanding of interrelated industrial decisions in the context of critical metals.

3.3. Environmental risk assessment

The explicit modelling of the socio-technical system will result in a distribution of outputs (e.g. material requirements) under certain scenarios. In combination with environmental impacts across the life cycle of metals, those distributions allow for an evaluation of environmental risks related to industrial substitution decisions. Compared to previous approaches this is again a more explicit evaluation of potential environmental implications, however it bares the risk of undermining accepted life cycle assessment insights with modelling uncertainties.

3.4. Addressee

With the exception of Graedel et al. (2012), current approaches assessed the criticality of metals for whole industrial sectors or countries. The approach proposed here focuses on single industries or even companies. This allows a customized criticality assessment for industrial stakeholders on the one hand, but limits the transferability of results on the other hand.

3.5. Scope

The explicit dynamic modelling of industrial actors' behaviour and its consequences on the material flows and criticality of metals at stake clearly limits possible scopes of the approach. While the coupled model would allow highly context specific criticality assessment, cross-insights to other industries and/or elements are limited.

4. Conclusion and outlook

In this paper we proposed an approach to evaluate the criticality of raw materials that goes beyond the current state of the art in the sense that it explicitly includes the dynamic interrelations between industrial substitution decisions and their implication on the criticality of metals considered. Our motivation for doing so was to stimulate research about dynamic criticality assessment tailored for industrial stakeholders, which we envision as an important addition to the criticality discussion in the future.

As such, the approach will allow simulation of dynamic market responses to substitution decisions as part of risk management strategy of industrial stakeholders. This will advance the understanding of supply risk significantly beyond the static indicator approaches currently proposed and enable a more systematic analysis of complex market responses. Although the prospective approach addresses rather specific industrial substitution decisions and their consequences, we encourage further research to start with a generic “proof of concept” aiming at an in-depth analysis of the additional insights gained through the approach.

Conflict of interest statement

None.

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