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Benefits of resource strategy for sustainable materials research and development

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ABSTRACT

Material and product life cycles are based on complex value chains of technology-specific elements. Resource strategy aspects of essential and strategic raw materials have a direct impact on applications of new functionalized materials or the development of novel products. Thus, an urgent challenge of modern materials science is to obtain information about the supply risk and environmental aspects of resource utilization, especially at an early stage of basic research. Combining the fields of materials science, industrial engineering and resource strategy enables a multidisciplinary research approach to identify specific risks within the value chain, aggregated as the so-called 'resource criticality'. Here, we demonstrate a step-by-step criticality assessment in the sector of basic materials research for multifunctional hexagonal manganite $YMnO_3$, which can be a candidate for future electronic systems. Raw material restrictions can be quantitatively identified, even at such an early stage of materials research, from eleven long-term indicators including our new developed Sector Competition Index. This approach for resource strategy for modern material science integrates two objective targets: reduced supply risk and enhanced environmental sustainability of new functionalized materials, showing drawbacks but also benefits towards a sustainable materials research and development.

1. Resource strategy

The global way of life is based on intensive consumption of energy and mineral resources. Many technologies with significant socio-economic benefits require materials that are problematic due to instable, insecure or price-volatile supply [1]. Moreover, the complexity of their global supply chains leads to an increasingly precarious scenario. The sustainable extraction and use of scarce natural resources are essential tasks to reach a resource efficient techno-economic development in the future [2]. The analysis of key technologies and processes of mega sectors shows their increasing dependency on availability of strategic metals and minerals, which is often limited [3]. The whole lifecycle (e.g. extraction, processing, pre-production, production, use-phase, recycling) of raw materials goes hand in hand with significant supply risks and environmental impacts. Applying criteria, like geologic availability, geo-political dependencies, ecological compatibility and reusability of novel materials along the complete material and product lifecycle are innovative and strongly recommended directions of materials science [4,5].

More precisely, in so called mega sectors [3] like the energy sector, high technology applications, e.g. as thin-film photovoltaic for power supply [6], supercapacitors for energy storage systems or power-to-gas technology for energy transformation, implement many different elements within their functional building blocks [7], demonstrating the complexity of its upstream value chain. Scarcities or upcoming restrictions of those strategic elements [1] for essential functions like cadmium telluride utilized as p-doped semiconductor adsorber layer for light-to-energy conversion in thin-film photovoltaic systems have a strong impact on the success of those products and technologies [8]. A challenging task for modern materials science is to develop high-performance materials utilizing abundant elements to replace critical ones in existing and future technologies [5,7,8]. Therefore not only technical material parameters are essential quantities, but also the identification of raw material restrictions or benefits. Often, criticality of elements is considered first at an advanced stage of product development [8–10], during end-of-life recycling scenarios [11,12] or the concepts include only specific aspects of materials efficiency [13] or raw materials supply [14–16]. Recent comprehensive criticality studies [3,17–19] consider in detail dimensions of supply risk, environmental implications and vulnerability to supply restrictions within global, national and corporate perspectives. However, for basic materials research at an early development

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stage the final product made by a functionalized material is not explicitly conceivable. Only mega sectors can be addressed for a possible future application.

Here, we specify a practical guideline for materials scientists to consider criticality aspects following a multidisciplinary evaluation for the use of raw materials. Indicators within the scope of reduced supply risk and enhanced environmental sustainability were identified from literature analysis [3,17,20,21]. These indicators were evaluated by experts from the fields of material science, physics, resource strategy and economics concerning their relevance within the basic research perspective, leading to a set of eleven indicators, listed in Fig. 2 (with details in tables S1 and S2 in the Supplementary Material). All indicators of this set have a long-term and forecasting perspective, contain non-redundant information and possess adequate data quality. The newly developed Sector Competition Index (SCI) comprises the predominant raw materials consumption in mega sectors accounting for the specific value added per material input. This multidisciplinary approach serves as a guideline for materials scientists for a sustainable and more resource-efficient material development. Here, it is based on a generation of reliable data containing geographically allocated reserves, production sites and resource supply dominating countries.

We illustrate the method on a multifunctional hexagonal manganite $YMnO_3$ [22]. This compound is a promising candidate for spintronics [23], non-volatile memory materials [24], domain-wall engineered multiferroic properties [25,26] at room temperature, or the direct electrically tuned exchange bias in $YMnO_3$/permalloy heterostructures [27]. These fascinating properties open new fields for future applications due to its geometrically driven improper ferroelectric ordering [28] accompanied by a structural six fold ferroelectric domain structure exhibiting topological protected vortices [29]. Recently, high dielectric constant and appropriate loss tangents at ambient temperature have been demonstrated in these materials, allowing good prospects for $YMnO_3$ to be also used as dielectric in high power capacitors for energy storage and conversion [30].

For $YMnO_3$, we focus on the basic research stage and assume a future “virtual usability” for this compound as a functional material in electronic building blocks. Due to the negligible amount of raw material required for research activities, restrictions concerning resource availabilities rarely occur already at this stage of product lifecycle, but may become an important factor in further development stages and technology spread. Our more simplified previous approach [5] for colossal dielectric constant materials demonstrated the benefits of knowing the criticality of the raw materials at this stage to prevent or even know risks in advance. For the present approach we derive the supply risk and environmental impacts of the two elements yttrium and manganese. The development of the supply risk indicators are discussed on an annual basis from 1995 to 2013.

2. Materials and product lifecycle

For the perspective of basic materials research a holistic approach is needed [31], especially taking into account long-term and forecasting criteria for raw material supply and production [3]. Therefore a multi-level product lifecycle for an implemented material is anticipated to identify development stages and upcoming risks based on raw materials usage. These risks are expressed by manifold indicators, which comprise technological [32], geological [33], geopolitical [14], economic [34,35], social [36] and environmental aspects [37]. The progress of a technology passes specific development stages from basic research to ready-to-use product, representing the resource-based approach of the material and product lifecycle. These stages are subjected to different disciplines like material sciences, industrial engineering, resource strategy and economics.

Within Fig. 1 we show a simplified view of various phases derived from the complex multidisciplinary and intersectional network of technology and product development: Basic research, technical development, application and re-phase. While basic research includes the conceptual functionalization of a material, in the technical development phases, the prototypical implementation for a specific product is carried out. Within the application phase the focus lies on production techniques for industrial upscaling as well as resource and energy efficiency aspects. Closing of material cycles across the whole material and product lifecycle is a necessity, thus closed-loop supply chains are established in the re-phase by recycling, remanufacturing and reuse [38,39].

The value chain in each level of Fig. 1 describes progress in material and product development (basic research and technology development) as well as industrial lifecycle (application and re-phase). Identification and classification of risks for all four lifecycle levels are prerequisite to develop risk mitigation strategies in order to achieve a sustainable use of functionalized resources. Many metals and metalloids show recycling rates below 1% [12]. Hence, there is potential for improvement in the design of industrial lifecycles, theoretically these materials can be recycled infinitely. Closing these material cycles would also allow for alternative material supply accompanied by reduced carbon emissions [40]. A detailed analysis of risks by combining efforts of a multidisciplinary research team, especially at the basic research level, can determine possible bottlenecks or benefits by functionalization of new materials early in a products lifecycle. A more resource-efficient use of scarce materials can be achieved or mitigation strategies developed. It is of high interest to compare criticality scores derived by this long-term approach with future criticality assessments of the same materials utilized in novel products.

Material scientists could use existing criticality assessments for a first estimate. However, all existing studies provide limited information for long-term developments. E.g. the broad coverage of metals and metalloids by Graedel and colleagues comes at the cost of only two supply risk indicators in the long-term perspective (depletion time and companion metal fraction) [18]. Other assessments either have a short- to medium-term perspective [41], a national focus [42] or only applied their method to a small set of raw materials. Therefore, we present a guideline for basic materials research on an international scale emphasizing long-term indicators.

3. Criticality assessment

3.1. Guideline for criticality assessment in basic research

The step-by-step guideline for a resource strategy in materials science is displayed in Fig. 2, which represents in more detail the basic research level of Fig. 1. It focuses on reliable information that is accessible for material scientists. The guideline starts with an analysis of the research material requirements for the desired function and the corresponding value chain (A). The second step implements analyses of data on raw material concerning data availability and quality (B), with consideration of geographically localized information for all risk indicators. Suitable risk mitigating solutions can be assessed by calculating these indicators in the supply risk and environmental perspective (C). A detailed description for calculation of each indicator is provided in the Supplementary Material (Table S1 and S2). The guideline finishes with an interpretation and conclusion.

3.1.1. Value chain (A)

Initially, material scientists need to become aware of material demands concerning aspects of purity of raw material or manufacturing techniques within preprocessing, in order to address inter alia specific environmental impacts or market concentration. Data analysis is either carried out on a global level or has a regional focus. For this purpose, data sources for the various indicators include scientific journal articles (like metal recycling rates [12,43]), administrative institution reports (like USGS [33]) or proprietary consultant information (like SNL Metals & Mining [44]). If necessary, data gaps can be closed by consulting a resource strategy expert.