



Development and application of screening-level risk analysis for emerging materials

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ABSTRACT

Analysis of a material's impact on society is increasingly recognized as a necessary step in materials development, especially in the area of lead-free piezoelectrics. Evaluations of the environmental, health, and societal impacts that occur throughout the material's life cycle are critical for determining the viability of lead-free alternatives. Risk screening approaches, such as the screening-level Emerging Materials Risk Analysis (EMRA) proposed in this work, may help researchers compare materials or material production routes to determine more sustainable solutions. As a first demonstration of its utility in the development of lead-free piezoelectrics, the approach introduced in this paper is applied to piezoelectric HfO₂ (hafnia) to compare mining and processing routes and to elucidate the more sustainable route for HfO₂ production. This paper aims to exemplify how the EMRA risk screening approach incorporates perspectives on environmental, health, and societal impacts into the materials research process by providing a relative risk screening evaluation of different material processing routes and/or different materials. Results from applying EMRA to hafnia show that the major known environmental impacts of hafnia mining and processing involve ecosystem destruction and heavy use of fossil fuels and electricity; health impacts related to potentially unsafe working conditions and potential exposure to radioactive elements; and societal impacts including land disputes and supply concerns. Results also demonstrate that the more sustainable production route currently available includes commercial wet mining with land rehabilitation followed by beneficiation via wet processes with consistent personal protective equipment use and water recycling. Almost all of the previously-mentioned impacts are avoided in this life cycle route. Outcomes from this analysis identify hafnia as a potentially sustainable replacement for certain applications of PZT and therefore encourage continued development of the material. Future efforts will test EMRA on a wide variety of other materials and revise the approach accordingly.

1. Introduction

New and existing materials are advancing faster than ever with the advent of materials development technology. With the growing field of materials informatics, machine learning models can generate a mass of new materials much faster than traditional trial-and-error methods, such as in the case of superconductor development [1]. However, the idea of sustainable materials development, defined here as recognizing and actively minimizing the potential environmental, health, and societal consequences of material use, has also become increasingly relevant. For example, the International Risk Governance Center (IRGC) recently identified that not enough attention is paid to climatic and

environmental risks related to emerging technologies and suggest that more work is needed to develop prospective life-cycle based tools that can help make decisions towards sustainability when there is limited data and heightened uncertainty to advance design in more sustainable directions [2]. Balancing the rapid development of new technologies with conscientious design is a challenge, especially when the evaluation of long-term consequences is time-consuming and costly and it can be difficult to translate the well-defined idea of sustainability into practical assessment tools [2]. Further challenges are presented by the existence of competing objectives (e.g. material performance, cost, sustainability) and dissimilar opinions about optimal solutions from different stakeholder perspectives.

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One criticism regarding the application of traditional, quantitative assessments to evaluate the human health and environmental impacts of materials such as Life Cycle Assessment (LCA) is that these methods are typically conducted in later design stages or even post-commercialization rather than within early research, development, or design phases, making sustainability an afterthought in material development, design, and use [3]. This is because the development of materials is often guided by the design requirements of a larger system (e.g. function or performance of the material) and the intrinsic material parameters themselves despite factors such as supply risk and environmental impact of resource acquisition playing large roles in the long-term viability of material choice [4,5]. Prioritizing properties over sustainability has often occurred using traditional innovation models, particularly in cases where the amount of material required for research is low or negligible. However, it is increasingly recognized that life cycle impacts and sustainability factors need to be considered within early innovation cycles in order to avoid unwanted or unintended effects on health, environment, and society, following principles of responsible innovation [6]. To aid with proactive assessment of material sustainability, scholars evaluating emerging risks of technologies and advanced materials have urged the creation of new methods for assessing risk early on [7]. In this case, potential risks to human health (including occupational health and safety as well as consumer risks) and the environment have been a central focus, with additional considerations of ethical, legal, and societal risks related to the development and use of advanced materials. In recent years, there has been increased attention to safe-by-design (SbD) and anticipatory LCAs, with a growing number of SbD and LCA studies described as prospective, early stage, ex ante, anticipatory, and explorative [3,8]. Given that there are currently a number of barriers to implementing responsible innovation in practice at institutional levels [9,10], materials science researchers and innovators may be in better positions to kickstart sustainable materials development by making informed decisions in the early innovation stages, thereby greatly influencing the sustainability of future applications and devices. This approach may be particularly important in order to achieve circular economies [11]. Existing design principles that have been applied to make material production inherently safer include substitution of hazardous reagents or materials and attenuation of particularly dangerous operative conditions such as temperature and pressure [12,13].

One area of research where sustainable materials development activated by researchers could be especially useful is in the development of lead-free piezoelectrics. Piezoelectrics are electronic materials that exhibit a mechanical strain response to an electrical field or a dielectric displacement (i.e., charge) in response to mechanical stress [14,15]. Piezoelectrics are found in motors and generators and are a key component of sensors, transducers, and actuators [15,16]. Moreover, the market for piezoelectrics is projected to grow from the current \$28.9 billion to \$34.7 billion over the next five years [16]. Lead-based piezoelectrics such as lead zirconate titanate (PZT) have proved an important player in the piezoelectric market due to their strong piezoelectric performance in such a wide breadth of applications [17]. Legislative policies such as the European Union's Restriction of Hazardous Substances (RoHS) heavily restricts or bans the use of several materials including lead (Pb) in electrical and electronic equipment [18]. The RoHS aims to minimize the amount of lead that can enter the environment via production and disposal of electronic devices. As a result of the RoHS legislation, there has been increased interest in finding lead-free replacements [17]. Though lead-based piezoelectrics currently have an exemption to the RoHS ban as there are not yet robust enough alternatives to PZT for widespread use in industry, it is possible that the exemption could be lifted when commercially-robust, lead-free piezoelectric alternatives emerge. However, in order for the exemption to be lifted, the environmental, health, and in some cases societal and economic costs of the alternative material must not be greater than those of PZT [17].

To date, the environmental costs of two lead-free alternatives to PZT have been evaluated [19,20]. Potassium sodium niobate (KNN) and sodium bismuth titanate (NBT) were assessed using ISO-standard Life Cycle Assessments (LCAs) at a later stage in their development. It was found that neither material offers "absolute competitive edge from an environmental perspective in comparison to PZT" [20]. While an LCA gives extensive quantitative results that are easy to compare, completing an LCA can cost around \$50,000 per product (and in some cases, more), take several months to complete, and often requires some amount of expert knowledge to perform [21]. Furthermore, LCAs are highly technical in nature and difficult for non-specialists to interpret, making them poor guides for decision-makers outside of the LCA field [22]. LCA proponents stress the importance of utilizing an LCA to inform decisions early on in the material development process [23], though LCAs are inherently difficult to implement in the early stages of material development where funding for sustainable analysis is low and time is of the essence. It is neither practical for researchers actively engaged in materials development nor reasonable to perform on all possible emerging materials. With the growing piezoelectric market [16] and the call for increased development of alternative lead-free alternative materials, sustainability concerns may not be fully prioritized due to competing demands.

A screening-level risk analysis approach, which may be more cost- and time-effective and be performed by researchers without expert knowledge in LCA during the earlier stages of material development to capture environmental, health, and societal perspectives, could help focus development on materials that are safe(r) and more sustainable. Here, "safe" refers to the absence or minimization of harm to human health or the environment, and "sustainable" refers to the triple-bottom line approach that considers health and environmental, social and ethical, and techno-economic considerations. Screening-level approaches may be more practical than carrying out full RAs and LCAs, especially as a first-step in the research process when trying to decide which material or production route is more sustainable. Such safe and sustainable materials development is an iterative process, allowing for development directions to continually shift with the acquisition of new information [24,25]. Additionally, screening level risk analysis tools are especially suited for use in early development stages as they can use readily available information to help guide short-term decision making, such as in the ideation and preliminary assessment stages within the Stage-Gate system where a project follows stages from ideation to launch, with gates serving as decision points to proceed, review and revise, or discontinue the project [26]. Using screening level risk analysis tools in early development phases may be particularly critical in materials development when decisions may need to be made faster than comprehensive analyses, such as LCA and risk assessment, can allow. We also note here that screening-level risk analysis tools are not intended to fully substitute applications of RA and LCA, which may be important and effective tools to quantify risks and impacts across life cycle stages; rather screening-level analyses are intended to serve as a first-step towards understanding potential impacts of a material or process using less resource-intensive approaches than required by applications of RA and LCA.

The approach presented in the paper, henceforth called the Emerging Materials Risk Analysis (EMRA) screening approach, is a relative risk screening evaluation that compares and contrasts different materials or life cycle paths of a single material to aid researchers in short-term decision making during the process of developing new and emerging materials. It incorporates life cycle thinking and risk screening in an attempt to methodize early-stage sustainability assessment, which the IRGC has identified as essential for guiding sustainable design of emerging technologies [2]. Similar to traditional LCA, the EMRA is based on an impact analysis of a material throughout its life cycle, though it relies on screening-level evaluations rather than in-depth quantitative assessments. The approach was inspired by integrating aspects of existing hybrid LCA and Environmental Risk Assessment (ERA)

approaches [27–32] as well as more specific tools developed to evaluate nanomaterial health and environmental risks (e.g. Nano Life Cycle Risk Assessment (LCRA), LICARA nanoSCAN, NanoRiskCat, GUIDEnano), which have been proposed as alternatives to ISO standards and are specific for assessing nanomaterials along with many other tools and frameworks [33,34]. It also incorporates elements of approaches used to make decisions across life cycle stages, such as the Multi-Criteria Decision Analysis (MCDA) [35]. The EMRA screening approach is suitable for relative risk screening to compare any material(s) or processes, though it is especially suited for emerging materials in situations where there is incomplete data. Further, the EMRA approach may serve as a precursor to a more elaborate life-cycle analysis by allowing researchers to identify and consider the entirety of known environmental, health, and societal impacts in the early stages of materials development. Unlike traditional LCAs which are costly and time consuming, the EMRA approach can be implemented with access to standard academic databases and peer-reviewed literature and requires no specialized knowledge of the LCA field.

To demonstrate the utility of the EMRA screening approach, we assessed thin-film HfO_2 (hafnia), a rapidly-emerging lead-free piezoelectric material. Thin-film hafnia is an example of a newly discovered material whose environmental, health, and societal impacts are understudied. While hafnia had been previously deployed by Intel® in the semiconductor industry for its high-k dielectric applications [36], a surge of new exciting applications emerged after ferroelectricity in thin film hafnia was reported in 2011 [37]. Ferroelectrics, a subclass of piezoelectrics, have gained popularity in the electronics field where applications such as non-volatile memory, energy harvesting, electrocaloric cooling, and neuromorphic computing have been investigated [38–42]. Aside from its originally unexpected ferroelectric properties in thin film form, its lead-free composition has garnered increased attention in the past decade.

This research paper therefore describes the design of the novel Emerging Materials Risk Analysis (EMRA) approach, as well as its application to direct the development of hafnia as a lead-free piezoelectric material. We also discuss the main findings for the sustainable development of hafnia and provide a critical examination of the approach and future prospects. In this discussion, we note that this paper reports on the first version of EMRA and its application to hafnia materials, with the intention of further revising and refining the approach in subsequent versions.

2. Materials and methods

2.1. Overall structure of the emerging materials risk analysis (EMRA) approach

The Emerging Materials Risk Analysis (EMRA) is a relative screening-level approach intended to help identify environmental, health, and societal risks that may occur along a material's life cycle. As a relative risk screening approach, it can compare alternative materials or material production routes to help inform decision-making regarding the most sustainable way to proceed. However, due to its simple qualitative evaluation, it can only be considered a short-cut preliminary evaluation tool and does not replace more robust quantitative tools that should be applied later on in the decision-making process. The EMRA was developed by examining peer-reviewed manuscripts and reports on materials sustainability, life cycle assessment, risk assessment, and risk analysis. Special attention was given to approaches used to evaluate and make decisions regarding engineered nanomaterials and other advanced materials, as several different risk assessment and risk analysis tools and frameworks have been recently developed to assess risks of nanomaterials and advanced materials over life cycle stages [28,33–35,43–45]. After reviewing the literature, we identified key aspects of risk analysis frameworks to include in the EMRA so it could evaluate potential risks of emerging materials throughout the material's

life cycle.

Following established life cycle-based evaluations [46], we identified four main life cycle stages to be examined by the EMRA: 1) obtaining raw material, 2) processing the material (which includes all material processing from mineral beneficiation to fabrication and deposition techniques), 3) use of the material, and 4) disposal of the material. Potential impacts in each life cycle stage were investigated in regard to environmental, health, and societal impacts. We chose to focus on these three types of impacts because they were deemed especially important for consideration during the sustainable development of a material according to the RoHS Directive [18]. Economic factors were not explicitly considered by the EMRA as they can be effectively analyzed using tools such as cost-benefit analysis or techno-economic assessment, as discussed further in Section 4.

The EMRA consists of five phases: 1) defining the goal, scope, and scenarios, 2) collecting relevant data and information on the material's life cycle, 3) organizing collected data and information into a impact table and life cycle flow chart, 4) performing risk analysis using risk matrices or tables, and 5) drawing conclusions and addressing uncertainty. Each step is visualized in Fig. 1 below, with more details outlined in Sections 2.2.1–2.2.5. Due to the nature of largely qualitative analysis, special care was taken to indicate and minimize potential sources of bias when possible, as described below.

2.2. Guide to using the EMRA

2.2.1. Defining the goal, scope, and scenario(s)

Intentional goal-setting is crucial for efficiently employing the EMRA in materials research and design. Project goals are identified by thinking about what purpose the approach serves with respect to the researcher's needs. The EMRA is an adaptable decision-making tool based on evaluations of potential risks and impacts and can be used to accommodate a range of different goals. For example, a researcher trying to choose between potential materials to use in a design phase could have a goal to determine which material has the lower/lowest associated risk(s). A researcher may also want to determine the best route for mining and/or manufacturing a given material to inform their choice of supplier. The EMRA should be used for comparative analysis, e.g., comparing different materials or processing routes, and does not aim to replace quantitative risk assessments for individual materials.

Defining the scope and boundaries is a common practice in many forms of risk assessment including in the LCA method [23]. Setting a project goal and scope helps establish the system boundaries and begins with outlining the process steps and stating assumptions. Defining the scope also involves considering both the material (e.g. the entire device or a specific material in the device) and the relevant parts of the life cycle (e.g. the entire cycle–cradle-to-grave, or only the manufacturing steps–cradle-to-gate).

The EMRA uses the goal and scope of the project to define different risk scenarios. A scenario in this text refers to the specific life cycle route. Specific assumptions regarding each scenario should be clearly stated along with transparent reasoning about why the researchers believe the chosen scenarios are realistic and valid choices for analysis (i.e., that the scenarios are reasonably plausible, accurate, culturally relevant, and based on current information). Multiple scenarios can be considered for a single material because there are many ways to obtain, process, use, and dispose of a single material. Choice of scenarios allows the researcher to cater the risk analysis to their goal. For example, a researcher can compare their lab-specific processing route for a material with alternative routes available in literature. More generally, it is possible to compare all of the different possible scenarios that could create a material to determine an objective best and/or worst way to go through the route to draw general conclusions about the overall life cycle of the material.

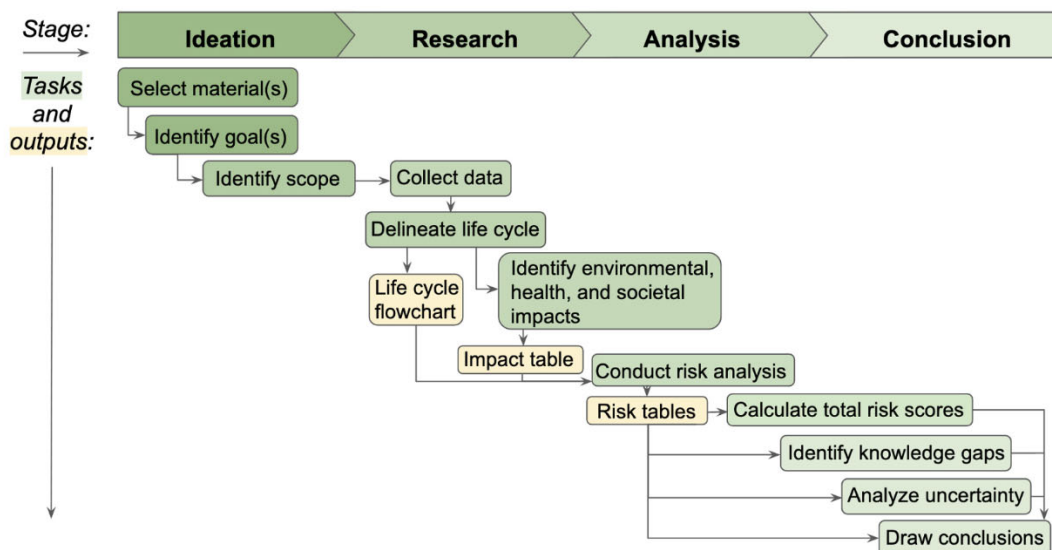


Fig. 1. Schematic representation of the stages of the emerging materials risk analysis (EMRA).

2.2.2. Data and information collection

Once the project goals and scope are determined, the next step in EMRA is to investigate existing information on the life cycle and impacts of the selected material. In our own application of the EMRA screening approach, a literature review was performed using primarily publicly-available literature found through scientific search engines. Generally, the extent of the investigation will depend on the time and resources at the researcher's disposal as well as self-determined parameters that the researchers deem important to assess within the scope of their project, e.g., environmental risk, human health, political stability, etc. Since the risk analysis depends largely on the choice of sources, the researcher should describe search terms, databases, etc., as well as what they have chosen to include and discard certain information. Throughout the research process, one can also track and assess the reliability of the sources where information is obtained from.

The EMRA is intended for emerging materials and/or quick decision-making; if ample information and resources are discovered during the data collection process, the researcher may consider a more robust quantitative approach such as LCA.

2.2.3. Life cycle flowchart and impact table

Information about the general life cycle of the material is then used to construct a life cycle flowchart (e.g. Fig. 3 in subsection 3.1). The life cycle flowchart delineates the known life cycle of the material and identifies instances of environmental, health, or societal impacts using symbols. The flowchart visually indicates the scope of the study and highlights the uncertainty present in each step of the life cycle. Scenarios chosen for risk analysis are shown in the life cycle flowchart by highlighting the exact route through the life cycle of the material each scenario pertained to (see Fig. 4 in subsection 3.3). Some information (e.g., processing and mining details) may be proprietary and thus not available in the literature. Care should be taken to indicate any discontinuities between processing steps due to data unavailability. Further, the option to indicate which steps are within the scope of the study allows the researcher to clearly communicate what risk was being considered.

An impact table (e.g. Table 3 in subsection 3.2) is then made to summarize all qualitative and quantitative data obtained relevant to each impact criterion (environmental, health, societal) in each of the four life cycle stages (obtaining raw material, processing of the material, use of the material, and disposal of the material). The impacts are instances of environmental, health, and societal impacts along the material's life cycle. All possible impacts from all scenarios should be listed in the impact table. The sources that report each impact are listed next to

the corresponding method. Further guidance on how to identify important environmental, health, and societal impacts from the material's life cycle can be found in the Supplementary Information (SI). Applying EMRA to different materials or under different scenarios may require adapting the underlying data and information to the material/scenario in question. For example, some users may wish to focus the EMRA analysis specifically on understanding potential risks on certain life cycle stages or processes or with a unique focus on e.g. worker health, among others.

2.2.4. Risk matrices or tables

Using the impacts outlined in the impact table, risk matrices or tables are then generated for each relevant scenario. Each impact is assigned a risk score based on its respective consequence and probability, and the risk scores are added to determine the overall (relative) risk for the given scenario. Example risk tables can be found in subsection 3.3.

A derivative of the Fermi National Accelerator Laboratory (Fermilab) Prevention through Design (PtD) risk matrix (see Fig. 2) is used to determine the risk scores for each impact [47]. The PtD risk matrix was selected for use in the EMRA since it leveraged previous studies and investigations related to safety by design [48]. There are separate fields of study that investigate potential human health risks from exposure to various substances (e.g. toxicology) which are related to but distinct from fields of study that focus on occupational health and safety. For the

		Consequence				
		Minimal	Low	Medium	High	Critical
Probability	A Almost certain	3	4	5	5	5
	B Likely	2	3	4	5	5
	C Possible	2	3	3	4	5
	D Unlikely	1	2	3	3	4
	E Rare	1	1	2	2	3

Fig. 2. PtD risk matrix adapted from Fermilab [47].

purposes of this study, the EMRA approach includes an overarching category of ‘health’ impacts that includes, but is not limited to, occupational health and safety. This focus on health goes beyond occupational health and safety but is based on previously-developed criteria provided by the Fermilab, which was included in this study due to our focus on screening emerging materials.

As shown in Table 1, the matrix considers both the severity of the impact (“consequence”) and likelihood that the impact will occur (“probability”). The consequence of each impact is rated as having “critical,” “high,” “medium,” “low,” “minimal,” or “unknown” severity as determined with reference to Table 1. The probability of an impact is considered “almost certain,” “likely,” “possible,” “unlikely,” or “rare” as determined with reference to Table 2. Both Tables 1 and 2 were based on previously-developed work from the Fermilab [47].

To determine the risk score of each impact identified in the previously-created impact table, Tables 1 and 2 are used to assign consequence and probability scores for each listed impact. Using the consequence and probability scores assigned for an impact, the risk score for the corresponding impact is then calculated using the PtD risk matrix in Fig. 2. The risk scores are shown as numeric values in the risk matrix, corresponding to risk levels 1–5. If either the consequence or probability of the impact is considered indeterminate, a risk score should not be assigned and the risk should be labeled “inconclusive” for that impact. As risk scores are assigned, the consequence, probability, and corresponding risk score (if determinable) for each impact should be added to the risk table. A new risk table is generated for each scenario identified for risk analysis.

The final step for individual scenario risk analysis involves using the risk table to assign a total risk score. The total risk for a scenario is calculated by summing the risk score for each row in the risk table. For rows with an inconclusive risk score, a range of risk is calculated instead of a single total risk score by assuming the best and worst case scenario for each inconclusive row. Consequently, the range of risk is then the lowest possible risk associated to the highest possible risk associated with the given scenario. Additionally, a final column is added to the risk table to summarize brief conclusions for each impact. The conclusions can indicate whether or not a knowledge gap led to an inconclusive result, explain a low risk score, or suggest future work regarding the specific impact. If necessary, a “notes” column can also be added to the table to track the rationale for why a certain component was scored in a specific way or to note considerations relating to diverging findings.

Care should also be taken to minimize potential bias in determining the consequence and probability of each impact. Applications of EMRA may benefit from compiling data and information from a range of sources to estimate potential consequences and probabilities in order to capture variability between studies. Further, data gaps and sources of uncertainty can also be compiled in the literature review stage when applying EMRA in order to better understand the role of uncertainty in risk screening, as discussed in the next section. In addition, applications of EMRA should be transparent with processes used to assign risk scores based on the available literature, which will also help justify the risk scores in the analysis.

2.2.5. Analysis of results and uncertainty considerations

Once risk tables are constructed and the total risk score is calculated for each identified scenario, a relative risk ranking exercise can be used to identify the comparatively “most” and “least” risky options. Depending on the researcher’s goals, the risk ranking could lead to anything from prioritizing development of the lowest-risk material option to selection of a raw material supplier that utilizes the lowest-risk acquisition route. While it can effectively support comparative decision-making, the EMRA should not serve as an ultimate, universal risk screening of a material or scenario. The EMRA is intended to be used for initial decision-making between defined options using a time- and cost-efficient process.

To add perspective regarding the certainty of the judgment-based

Table 1

Consequence severity table modified from Fermilab [47] which includes examples of environmental, human health, and societal impacts.

Severity	Environment	Human health	Societal
Critical	Permanent loss of a natural resource or ecosystem (e.g. drinking water source, forest, air, river, mountain).	Multiple deaths from injury or illness; multiple cases of injuries involving permanent disability; or chronic irreversible illnesses.	Willful disregard for the law, loss of multiple public land sites or multiple community facilities (valued at >\$5,000,000), severe infringement on the rights, liberties, or equal opportunities of most community members, and/or loss/shut down of a community program or project.
High	Long-term loss of a natural resource or ecosystem (e.g. drinking water source, forest, air, river, mountain).	One death from injury or illness; one case of injury involving permanent disability; or chronic irreversible illnesses.	Major noncompliance with the law that could result in fines and penalties, loss of a public land site or a community facility (valued at >\$5,000,000), major infringement on the rights, liberties, or equal opportunities of most community members, and/or major impact to the budget or schedule of a community program or project that could jeopardize program operation or project completion.
Medium	Seriously impairs the functioning of a natural resource or ecosystem.	Injuries or temporary, reversible illnesses resulting in hospitalization of a variable but limited period of disability.	Major noncompliance with the law that could result in a report to authorities, major damage to a public land site or a community facility (value of damage between \$1,000,000 - \$5,000,000), significant infringement on the rights, liberties, or equal opportunities of many community members, and/or significant compromise to the budget or schedule of a community program or project that exposes program or project to potential failure if gap cannot be immediately resolved.
Low	Isolated and minor, but measurable, impact(s) on some component(s) of a natural resource or ecosystem.	Injuries or temporary, reversible illnesses not resulting in hospitalization with lost time.	Programmatic noncompliance with community standards, minor damage to a public land site or a community facility (value of damage between \$50,000 - \$1,000,000), minor infringement on the rights, liberties, or equal opportunities of many community

(continued on next page)

Table 1 (continued)

Severity	Environment	Human health	Societal
Minimal	No measurable impact on component(s) of a natural resource or ecosystem.	Injuries or temporary illnesses requiring only minor supportive treatment and no lost time.	members, and/or minor impact to the budget or schedule of a community program or project that does not significantly compromise the program or project. Specific instance of noncompliance with community standards, minor damage to a public land site or a community facility (value of damage <\$50,000), minor infringement on the rights, liberties, or equal opportunities of some community members, and/or minor impact to a community program or project that does not compromise the budget or schedule of the program or project.

Table 2

Impact probability table adapted from Fermilab [47].

Probability	Description
A - Almost certain	Could occur annually
B - Likely	Could occur once in two years
C - Possible	Occurring not more than once in ten years
D - Unlikely	Occurring not more than once in thirty years
E - Rare	Occurring not more than once in one hundred years

analysis, uncertainty considerations are also included in EMRA. An uncertainty level of “high,” “moderate,” or “low” is qualified for each impact and listed next to each individual risk score in the risk table. The method for determining the uncertainty level is qualitatively assigned by the researcher, though it is suggested that the researcher should choose a common metric on which to base the uncertainty analysis. For example, uncertainty may be judged based on the availability and/or quality of data/information, frequency of conflicting findings, or expert judgment. The researcher should also state the strategy used for determining uncertainty. Whenever possible, the researcher should try to base judgment on an external metric (e.g. number of sources, journal impact factor, number of source citations, etc.) as this helps quantify judgment more objectively.

An overview of the entire process of completing the EMRA is shown in Fig. 1 in Section 2.1. After completion of the EMRA, the findings should be revisited periodically as more information becomes available.

2.3. Application of the EMRA to hafnia thin films

Specific details regarding the process of applying EMRA to analyze hafnia thin films are included below. The goal of the hafnia case study was to determine which of four common cradle-to-gate life cycle routes for making thin film hafnia from heavy mineral sand is more sustainable or least impactful across environmental, health, and societal parameters. To assess the potential impacts that occur along the hafnia life cycle, a literature review was conducted by a keyword search in scientific databases (e.g. Web of Science) related to hafnium metal mining and beneficiation and hafnia thin film deposition methods. Peer-reviewed

papers, reports, and dissertations were used as main sources.

Once information about the life cycle and potential impacts was collected, a life cycle flowchart was created to visualize the four different life cycle routes. The steps involved in each of the four considered life cycle routes are highlighted in the relevant sections of the life cycle flowchart (see Fig. 4 in subsection 3.3 and Figs. S1-S4 in SI). The assumptions corresponding to each life cycle route were detailed (see SI). Four risk analysis tables (Tables 4–7) were then constructed based on the chosen routes. Impacts were listed in each applicable risk table. When there was no impact information found for a specific criterion in a life cycle stage, “none found” was recorded. In the hafnia thin film case study, uncertainty related to each impact was indicated by the number of sources that corresponded to each impact claim.

2.4. Study limitations

While the EMRA approach has a number of strengths, including a more time- and resource-efficient approach to risk-screening of materials, we also recognize that there may be a number of limitations. First, the EMRA approach intends to provide a risk-screening evaluation rather than to conduct a quantitative risk assessment and does not attempt to explore a comprehensive list of scenarios that vary in probability of exposure and severity of effects across health, environmental, and societal parameters. Relatedly, the EMRA approach focuses on broader categories of health, environmental, societal impacts, and does not necessarily concentrate on one dimension of risk, such as occupational worker health and safety. We note here that individual applications of the EMRA approach are largely guided by the researcher conducting the analysis: they could focus on specific materials, processes, or scenarios and the approach could also be modified for more in-depth aspects of occupational health and safety if needed by the user. In sum, researchers may wish to use the EMRA for an initial risk screening approach which can elucidate focus areas for a later quantitative risk assessment on select materials and life cycle flows.

Second, the EMRA approach is intended to serve as a relative comparison between materials or life cycle pathways in order to support decision-making. Therefore, the results are on a relative rather than absolute basis, similar to other decision-support approaches to compare alternatives (e.g. MCDA). Third, users may wish to revise an application of the EMRA approach in light of new or different data, similar to best practices in several nanomaterial risk assessment methods [33,49,50].

Finally, a more complete and conclusive study to promote full sustainable development of a material may wish to also incorporate stakeholder perspectives and needs. Presently, the EMRA only incorporates materials researcher perspectives; yet, there are many other stakeholders that may be involved in the decision-making process for sustainable material development, such as environmental and industry groups.

3. Results

The goal of the presented case study was to incorporate full life cycle sustainability into the future research and development of hafnia thin films by comparing and identifying the most sustainable of four common scenarios for hafnia mining and processing. To accomplish the goal, it was important to identify hazards that may arise during different life cycle stages. The scope of the study includes the most common routes for hafnium metal mining and hafnia thin film processing. The system boundary, most clearly visualized at the end of subsection 3.1 in Fig. 3, includes mining heavy mineral sand deposits, processing zircon via chlorination, deposition of the hafnia thin film on silicon via atomic layer deposition, and disposal of the hafnia thin film deposited on silicon. The functional unit is most relevant to the calculations in the thin film deposition step. The functional unit considered for the study is a 10 nm hafnia thin film deposited onto a silicon wafer with an area of 2.54

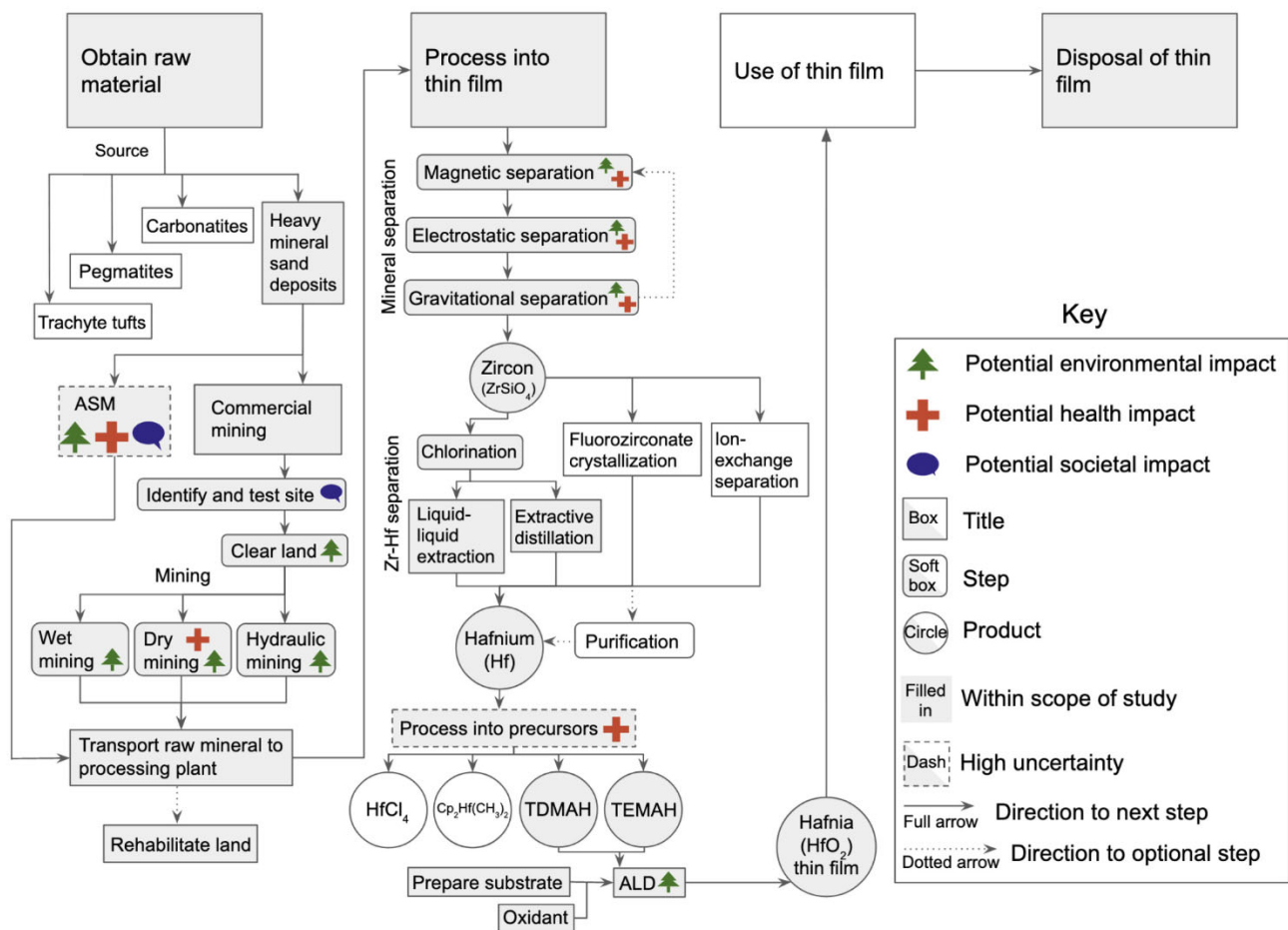


Fig. 3. Life cycle flowchart for hafnia thin films.

cm $\times$ 2.54 cm consistent with the dimensions of an average research sample in this field [51]. In reality, the size of a sample is often arbitrary and its dimensions are typically based on processing constraints such as the size and conformality of the ALD chamber, dimensions of patterning masks, size of the annealing chamber, and other post-processing steps. The 10 nm film thickness was selected because it is well-known that at this thickness regime surface energy effects preferentially stabilize the piezoelectric phase in thin film hafnia [52]. The following subsections provide more details about the life cycle of a hypothetical hafnia thin film. First, we provide an overview of the key life cycle impacts of hafnia thin films. For full details regarding life cycle stages of hafnia thin films, see Section 2 of the SI. We then analyze the potential environmental, health, and social implications of the impacts using the EMRA. Risks associated with different identified life cycle routes are calculated and compared to determine the more sustainable route for hafnia thin film production.

3.1. Overview of the life cycle of hafnia thin films

HfO₂ (hafnia) thin films have two primary constituents: hafnium and oxygen. Hafnium metal is most commonly sourced from zircon (ZrSiO₄) [53–55], where hafnium substitutes for around 2% of zirconium [53,54]. The most common natural source of zircon is heavy mineral sands [53–55]. The sands can be mined commercially or through artisanal and small scale mining (ASM). Once hafnium is extracted from zircon, it can be processed into precursor gases for the deposition of thin-film hafnia via chemical vapor deposition. After the films are deposited on the desired substrate, they are ready for use in additional post-processing, characterization, or disposal. A visual summary of the

life cycle of a hafnia thin film is shown in Fig. 3. More complete details about raw material acquisition, processing, use, and disposal can be found in the SI.

3.2. Identification of impacts through life cycle analysis of hafnia thin films using matrix

All identified environmental, health, and societal impacts resulting from the creation of hafnia thin films that were found in the literature review can be found in Table 3. The potential impacts occurring along the life cycle were identified based with reference to the EMRA Consequence Severity Table (see Table 1) as well as existing guidance on environmental, health, and societal hazard indicators [56,57] which is summarized in SI Section 1. To organize the information, each life cycle stage (i.e. obtaining raw material, processing of the material, use of the material, and disposal of the material) has been broken down into criteria (i.e. environmental, health, and societal) which are further broken down into individual impacts. References for each impact are listed in the rightmost column. The impacts are discussed in more detail in Section 2.2 of the SI, with the exact corresponding section listed under each criterion in Table 3.

3.3. Application of risk analysis to hafnia thin film case study

The goal of the case study was to compare different life cycle routes in order to determine the lowest risk processing route for hafnia thin films as well as highlight areas for future research. Four scenarios were analyzed: Scenario 1: commercial wet mining with land rehabilitation and beneficiation via wet processes with consistent PPE use and water

Table 3
Impact table for hafnia thin films.

Life cycle stage	Criteria	Impacts	References
Obtaining raw material (mineral)	Environmental (see SI: 2.2.1)	Destruction of ecosystem to mine heavy mineral sand - entire site must be cleared of plants, animals, and topsoil	[54,55,58,59,60]
		Heavy machinery fossil fuel use (e.g. diesel-powered trucks, excavators, dredges)	[54]
		Water use for mining (may need to be outsourced, could affect fertility of the soil)	[54]
		Unsafe working conditions (e.g. lack of protective gear, long hours in hot weather, child labor) in the case of artisanal and small scale mining (ASM)	[58,59,61]
	Health (see SI: 2.2.2)	Disputes over site use due to competing political, religious, or heritage claims	[59,60,61,62,63,64]
		Substantial electricity use required for mineral separation and atomic layer deposition (ALD) for thin film fabrication	[54], SI: 4.1
	Environmental (see SI: 2.2.4)	Emissions from mineral processing plants (e.g. CO, SO ₂ , and other toxic gasses)	[54,58]
		Potential exposure to concentrates of radioactive thorium and uranium when separating minerals	[54,55]
	Health (see SI: 2.2.5)	Volatile and flammable nature of ALD precursor powders - could be inhaled or spontaneously combust	[53,65,66,67,68]
		Material supply concerns (low recyclability, zirconium export requirements)	[55,69]
Beneficiation of raw material (mineral) + deposition of thin film	Societal (see SI: 2.2.6)	No suspected impact	[70]
		No suspected impact	[71,72,73]
	Health (see SI: 2.2.8)	No suspected impact	SI: 2.2.9
		No suspected impact	[63,69,74,75]
Use of material	Environmental (see SI: 2.2.10)	No suspected impact	[63,69,74,75]
		No suspected impact	[63,69,74,75]
Disposal of material	Health + Societal (see SI: 2.2.11)	E-waste - unregulated electronic waste recycling processes could impact health of those working at or near the site	[76,77,78,79]
		E-waste - unregulated electronic waste recycling processes could impact health of those working at or near the site	[76,77,78,79]

recycling, Scenario 2: commercial dry mining with no land rehabilitation and beneficiation via dry processes with no PPE use, Scenario 3: unregulated ASM and beneficiation via wet processes with consistent PPE use and water recycling, and Scenario 4: unregulated ASM and beneficiation via dry processes with no PPE use. These scenarios were chosen because they use the most common raw material source of hafnium, mineral separation steps, chlorination steps that are most common in the US, and precursors that are most commonly used in atomic layer deposition of hafnia thin films (see SI Section 2.1 for more details). The main differences between the scenarios highlight the range of risk resulting from sourcing the raw material from different types of mines and different processors that use varying amounts of safety equipment. In analyzing these different routes, the risks associated with researcher choice of material sourcing and manufacturing can be elucidated and compared.

The scenarios are outlined visually in Fig. 4 and shown distinctly in Figs. S1–S4 in the SI. Risk analysis tables were completed for each scenario. The scenarios were set up to demonstrate varying degrees of best practice implementation (with Scenario 1 having all best practices in place and Scenario 4 having the least amount of best practices in place) in order to demonstrate how different techniques can introduce or mitigate different degrees of risk.

Scenario 1: commercial wet mining with land rehabilitation and beneficiation via wet processes with consistent PPE use and water recycling had a cumulative risk score of 23–39. Calculations for the risk score of each of the four scenarios can be found in Section 4.2 of the SI. The risk analysis table for the given scenario is found in Table 4. The given scenario involved significant risk mitigation measures such as full rehabilitation of the mined land, utilization of wet processes whenever possible to minimize dust production (and recycling of water whenever possible), and proper use of PPE to minimize exposure to harmful materials, which contributed to its comparatively low risk score.

Scenario 2: commercial dry mining with no land rehabilitation and beneficiation via dry processes with no PPE use had a cumulative risk score of 28–47, which is higher than Scenario 1. The risk analysis table for the given scenario can be found in Table 5. Compared to Scenario 1, Scenario 2 saw an increase in risk mainly because the land was not rehabilitated, use of dry processes increased harmful dust production, and proper PPE was not used at all times.

Scenario 3: unregulated ASM and beneficiation via wet processes with consistent PPE use and water recycling had a cumulative risk score of 29–45, which is comparable to Scenario 2. The risk analysis table for the given scenario can be found in Table 6. Similar to Scenario 2, risk was increased because the land was not rehabilitated. Unregulated ASM also significantly increased potential health impacts as a result of unsafe mining conditions. Use of dry processes increased harmful dust production, and proper PPE protocol was not followed. In the beneficiation part of the life cycle, the utilization of wet processes to minimize dust production and use of proper PPE kept risk low.

Scenario 4: unregulated ASM and beneficiation via dry processes with no PPE use had a cumulative risk score of 33–52, which is the highest of the four scenarios analyzed. The risk analysis table for the given scenario can be found in Table 7. The high risk score is due to lack of land rehabilitation, unsafe working conditions due to unregulated ASM, increased dust from dry processes, and minimal PPE use.

A summary of the total risk scores for each scenario can be found in Table 8. Scenario 1 has the lowest total risk score as it incorporates all known safety measures. Future creation of hafnia thin films should attempt to follow a similar life route to reduce risk.

3.4. Determination of uncertainty levels in hafnia case study

As mentioned in Section 2.2.5, uncertainty surrounding the information heavily influenced the conclusions that were able to be drawn from each impact's risk score generated in Tables 4–7. The EMRA does not currently specify a basis for assigning uncertainty levels of “low”,

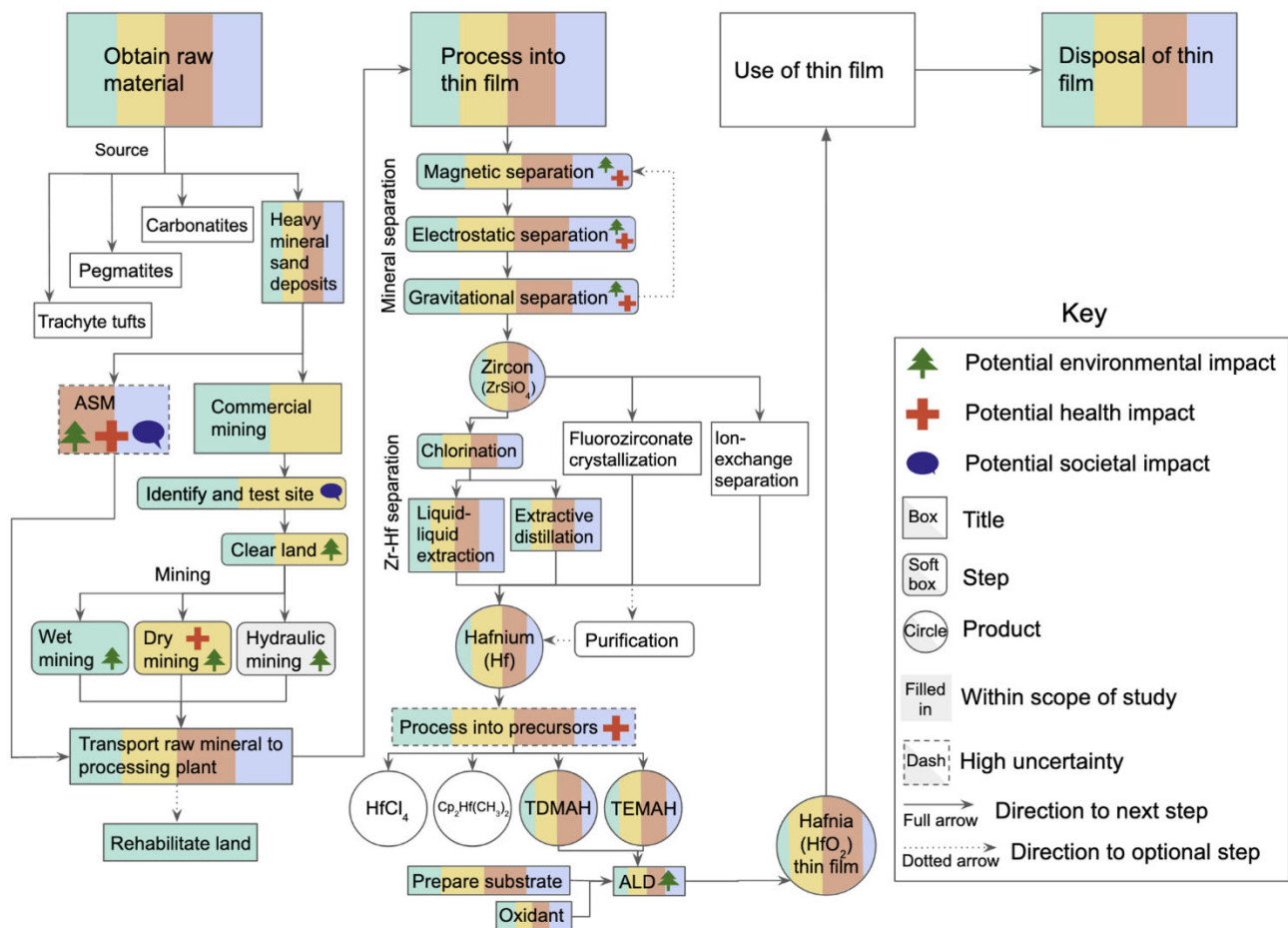


Fig. 4. Life cycle flowchart for different life cycle routes of hafnia thin films designated by different colors. Scenario 1: commercial wet mining with land rehabilitation and beneficiation via wet processes with consistent PPE use and water recycling (green), Scenario 2: commercial dry mining with no land rehabilitation and beneficiation via dry processes with no PPE (yellow), Scenario 3: unregulated ASM and beneficiation via wet processes with consistent PPE use and water recycling (red), Scenario 4: unregulated ASM and beneficiation via dry processes with no PPE use (blue).

Table 4

Risk analysis table for Scenario 1: commercial wet mining with land rehabilitation and beneficiation via wet processes with consistent PPE use and water recycling.

Impact	Consequence	Likelihood	Risk	Uncertainty	Conclusions
Destruction of ecosystem	Minimal	A - Almost certain	3	Low	Risk mitigated by land rehabilitation
Heavy machinery fossil fuel use	Indeterminate	B - Likely	Inconclusive	High	Data gap
Water use	Indeterminate	C - Possible	Inconclusive	High	Data gap
Disputes over sites	Indeterminate	Indeterminate	Inconclusive	High	Data gap
Energy use during ALD process	Medium	A - Almost certain	5	Moderate	Future research: how to decrease energy use in processing (or use other processing step)
Toxic gas created during extraction	Low	E - Rare	1	Moderate	More research may be needed to confirm low risk finding
Exposure to concentrates of radioactive material	High	E - Rare	2	Moderate	Risk mitigated by utilization of wet processes
Precursor powders are volatile and flammable	Medium	D - Unlikely	3	Low	Risk mitigated by PPE
Material supply concerns	High	Indeterminate	Inconclusive	High	More research into supply needed
Potential e-waste	High	Indeterminate	Inconclusive	High	Data gap

“moderate”, or “high”. In our application of the EMRA to the hafnia case study, we decided to base the level of certainty primarily on how many sources we found that mentioned the corresponding impact. Impacts described in 5–6 sources were given an uncertainty level of “low”, impacts described in 2–4 sources were given an uncertainty level of “moderate”, and impacts described in only one source were given an uncertainty level of “high”. Further, if the risk score was considered “indeterminate” because there was not sufficient information in the literature to assign the consequence or likelihood, the uncertainty level

was considered “high” regardless of the number of sources. For example, one of the most cited impacts was destruction of the ecosystem (see Table 3). As there were five sources that reported on the environmental destruction during hafnium mining, this impact received an uncertainty level of “low” in Tables 4–7. The conclusion drawn for this impact included a suggestion for risk reduction since there was enough data to suggest a sustainable way to minimize the hazard. On the other hand, the impact related to heavy machinery fossil fuel use was only mentioned by one source, giving it a “high” uncertainty level. The main

Table 5

Risk analysis table for Scenario 2: commercial dry mining with no land rehabilitation and beneficiation via dry processes with no PPE use.

Impact	Consequence	Likelihood	Risk	Uncertainty	Conclusions
Destruction of ecosystem	Critical	A - Almost certain	5	Low	Risk increased by improper treatment of land
Heavy machinery fossil fuel use	Indeterminate	B - Likely	Inconclusive	High	Data gap
Water use	Indeterminate	D - Unlikely	Inconclusive	High	Data gap
Disputes over sites	Indeterminate	Indeterminate	Inconclusive	High	Data gap
Energy use during ALD process	Medium	A - Almost certain	5	Moderate	Future research: how to decrease energy use in processing (or use other processing step)
Toxic gas created during extraction	Low	Indeterminate	Inconclusive	High	Data gap
Exposure to concentrates of radioactive material	High	B - Likely	5	Moderate	Risk increased by utilization of dry processes
Precursor powders are volatile and flammable	Medium	B - Likely	4	Low	Risk increased by disregard for PPE, suggested practices, etc.
Material supply concerns	High	Indeterminate	Inconclusive	High	More research into supply needed
Potential e-waste	High	Indeterminate	Inconclusive	High	Data gap

Table 6

Risk analysis table for Scenario 3: unregulated ASM and beneficiation via wet processes with consistent PPE use and water recycling.

Impact	Consequence	Likelihood	Risk	Uncertainty	Conclusions
Destruction of ecosystem	Medium	B - Likely	4	Low	Risk increased by improper treatment of land
Heavy machinery fossil fuel use	Indeterminate	C - Possible	Inconclusive	High	Data gap
Water use	Indeterminate	C - Possible	Inconclusive	High	Data gap
Unsafe working conditions	High	B - Likely	5	Moderate	ASM may substantially increase risk
Disputes over sites	Indeterminate	Indeterminate	Inconclusive	High	Data gap
Energy use during ALD process	Medium	A - Almost certain	5	Moderate	Future research: how to decrease energy use in processing (or use other processing step)
Toxic gas created during extraction	Low	E - Rare	1	Moderate	More research may be needed to confirm low risk finding
Exposure to concentrates of radioactive material	High	E - Rare	2	Moderate	Risk mitigated by utilization of wet processes
Precursor powders are volatile and flammable	Medium	D - Unlikely	3	Low	Risk mitigated by PPE
Material supply concerns	High	Indeterminate	Inconclusive	High	More research into supply needed
Potential e-waste	High	Indeterminate	Inconclusive	High	Data gap

Table 7

Risk analysis table for Scenario 4: unregulated ASM and beneficiation via dry processes with no PPE use.

Impact	Consequence	Likelihood	Risk	Uncertainty	Conclusions
Destruction of ecosystem	Medium	B - Likely	4	Low	Risk increased by improper treatment of land
Heavy machinery fossil fuel use	Indeterminate	C - Possible	Inconclusive	High	Data gap
Water use	Indeterminate	C - Possible	Inconclusive	High	Data gap
Unsafe working conditions	High	B - Likely	5	Moderate	ASM may substantially increase risk
Disputes over sites	Indeterminate	Indeterminate	Inconclusive	High	Data gap
Energy use during ALD process	Medium	A - Almost certain	5	Moderate	Future research: how to decrease energy use in processing (or use other processing step)
Toxic gas created during extraction	Low	Indeterminate	Inconclusive	Moderate	Data gap
Exposure to concentrates of radioactive material	High	B - Likely	5	Moderate	Risk increased by utilization of dry processes
Precursor powders are volatile and flammable	Medium	B - Likely	4	Low	Risk increased by disregard for PPE, suggested practices, etc.
Material supply concerns	High	Indeterminate	Inconclusive	High	More research into supply needed
Potential e-waste	High	Indeterminate	Inconclusive	High	Data gap

conclusion was that there may exist a data gap. Finally, the impact concerning site disputes was labeled “high” uncertainty since the risk was “indeterminate”, despite having six sources that mention the impact’s existence.

4. Discussion

4.1. Hafnia thin film findings

Analysis of hafnia using the EMRA indicates Scenario 1 (commercial wet mining with land rehabilitation and beneficiation via wet processes with consistent PPE use and water recycling) as the lowest risk processing route for hafnia thin films using the defined environmental, health, and societal risk criteria. Based on the current literature, it

appears that many key provisions from the life cycle route exemplified by Scenario 1 (e.g. commercial mining, rehabilitation of land) are commonly applied in Australian production of heavy mineral sands [80], but not necessarily applied in all heavy mineral sand mining endeavors globally. The least sustainable scenario was Scenario 4 (unregulated ASM and beneficiation via dry processes with no PPE use). The route introduced environmental risks because the land was not rehabilitated and health risks due to unsafe working conditions and potential exposure to harmful dust due to lack of PPE and control measures such as wet processing. Across all of the scenarios, the impact due to energy use for ALD contributed to a consistently high risk score of 5.

The four risk analysis tables identify areas for future research to ensure the most sustainable development of hafnia thin films. In particular, the consistently high risk score due to energy use in ALD

Table 8
Comparison of cumulative risk scores for each hafnia scenario.

Route	Risk
Route 1: > Mining - commercial, wet mining, land rehabilitation > Beneficiation - wet processes, max PPE used	23–39 Best practice
Route 2: > Mining - commercial, dry mining > Beneficiation - dry processes, no PPE	28–47
Route 3: > Mining - unregulated artisanal and small scale > Beneficiation - wet processes, max PPE used	29–45
Route 4: > Mining - unregulated artisanal and small scale > Beneficiation - dry processes, no PPE	33–52 Worst practice

processing indicates that future work should either focus on making ALD more energy-efficient or prioritizing other deposition techniques that require less energy. Further, it is possible that in scaling up the production of hafnia thin films, the relative amount of energy used to produce one functional unit would decrease. Future research should also be directed into closing the data gaps indicated by the tables. The magnitude of the environmental impact created by heavy machinery fossil fuel use and water use in the mining process is inconclusive, indicating data gaps. Additionally, there is a data gap regarding disputes over mining sites as the reports are anecdotal and the full extent of the impact is not known. The likelihood of impacts due to electronic waste is also a data gap. More research may also be needed to understand the prevalence of toxic gas during extraction to determine the extent of the environmental and human health risks. Considering missing data in the life cycle as a whole, the processing route for ALD precursors should also be assessed further to ensure there are no severe risks associated with precursor production.

In the context of sustainable development of piezoelectric materials, it is important to acknowledge that an ISO standard exists for application of a thorough life cycle assessment of materials and has been successfully applied to compare PZT, KNN, and NBT. As other developers of risk assessment methodologies acknowledge, not all materials under development can justify the cost and time commitment of a complete quantitative analysis, especially those that may involve inherent or intentionally-planned low risk [50]. As such, the EMRA should be used to identify which materials require costly quantitative risk assessment to aid in sustainable materials development and which materials need less information to make acceptably-informed decisions. The presented approach should not be considered a direct alternative to the ISO-standard LCA, but instead an approach that can be applied more readily and earlier on in the material development process than an ISO-standard LCA. Future work may include the development of a streamlined process for the incorporation of quantitative LCA data (such as the data from previously conducted LCAs on KNN, NBT, and PZT [19,20]) into the EMRA for comparison of risk scores between materials. Making the two methodologies compatible is key for ensuring the EMRA's utility in the ongoing lead-free piezoelectric materials development process.

4.2. Future development of the EMRA screening approach

The present paper reports the first version of the EMRA which can be further refined and revised in subsequent work. Future work with the EMRA screening approach could include more rigorous testing of the approach. First, it is important to have a range of users test out the framework on hafnia thin films using the same routes to confirm the findings. The approach could then be tested on other routes within the hafnia life cycle

and/or other materials. It is currently unclear how the EMRA will perform on non-hafnia materials since the approach has only been tested on hafnia. As previously mentioned, it may be useful to test the EMRA on piezoelectrics for which LCA data exists (e.g. KNN, NBT, PZT) to see if the EMRA can provide a similar comparison between materials. Testing the EMRA on other classes of emerging materials (e.g. nanomaterials, biotechnologies) could also help illuminate the applicability of the approach. Finally, assessment of the general EMRA approach and the conclusions drawn regarding hafnia by other materials researchers (especially in the piezoelectric realm), risk analysis specialists, and other stakeholders may also be useful to ensure the approach's robustness.

The uncertainty aspect of the EMRA screening approach could also be expanded upon with future work. Presently, the uncertainty aspect of the approach highlights areas that may indicate limitations of present knowledge about a material, such as significant limitations in data availability. In this way, uncertainty was mainly used to suggest directions for future research to fill identified data gaps. In the hafnia case study, the level of uncertainty for each impact was mainly determined by the number of sources that supported a specific claim. While a good starting point for the consideration of uncertainty, solely considering the number of sources that mention a claim is not a comprehensive approach to evaluating uncertainty. Future refinement of the uncertainty aspect of the EMRA may include taking into account the type of source (e.g., website vs. peer-reviewed article), the credibility of the source (e.g., the impact factor of the journal in which it was published, number of citations), and statistical or empirical support. Ideally, uncertainty should inform conclusions drawn from the present results by indicating how much weight should be put on results from each part of the EMRA analysis.

Another avenue for expansion of the EMRA screening approach is the incorporation of input from a broader range of stakeholders. For example, a stakeholder meeting specifically for the piezoelectrics community (including materials researchers, industry members, economists, etc.) could enhance the justification and applicability of the EMRA for future sustainable development of piezoelectrics. In the case of developing lead-free piezoelectrics, many of the problems that come with fully implementing a lead-free alternative such as hafnia have to do with difficulty in scaling the production [81]. Industry has yet to adopt PZT alternatives, in part, because lead-free materials are not commercially available and the cost and intellectual property concerns create significant barriers [17]. More generally speaking, incorporating economic and/or industry perspectives into the EMRA could help strengthen its feasibility as a decision-making tool. Recently, researchers have highlighted the need for convergence of materials science with social sciences such as economics to take a more holistic approach to understand why certain proposed technological solutions are not adopted by society [82]. Additionally, future supply may play into the economic viability of producing a material on an industrial scale [83]. To address the economic and industry concerns, future development of the presented approach could incorporate cost-benefit analyses and other economic analyses to address supply chain concerns [22].

5. Conclusions

While LCAs can provide thorough information about the environmental, health, and societal impacts of a material, they can be expensive, time-consuming, and challenging for an everyday materials scientist to complete. The proposed EMRA screening approach was developed to assist researchers in the early materials development stage and to inspire the development of materials that are inherently safe(r)-by-design. While the EMRA is not to be considered a thorough analysis of risk nor the panacea solution to sustainable materials development, it presents a relatively simple and less resource-intensive tool that may help researchers conduct screening-level assessments of their material(s) and possibly direct future work. The presented approach is time-efficient when applied to a given material or set of materials, as it can be

completed on the order of weeks instead of months to understand key environmental, health, and societal impacts that can be fed back into material selection and design phases. In other words, by applying the EMRA in the early stages of materials development, researchers will be able to create more sustainable solutions. The current study aims to develop the first version of the EMRA approach that can be further refined in subsequent versions. For example, a user may wish to tailor an application of EMRA to specific materials, processes, and/or to focus more on e.g. occupational health and safety compared to other impact categories (e.g. environmental risks). Further, the user is also able to expand uncertainty analyses to include more comprehensive assessments of uncertainty, based on the needs of the user. Nonetheless, this paper provides a first demonstration of the EMRA approach and its application to hafnia thin films.

When applied to the case study of piezoelectric hafnia, the EMRA approach is an essential first step in the consideration of hafnia as a promising lead-free piezoelectric. In the case of lead-free piezoelectric materials development, the EMRA approach can save researchers time and money in the search for a feasible, RoHS-compatible PZT alternative. A proactive approach would limit the need for the completion of full quantitative risk assessments on each novel material after they have been developed and can serve as a stage gate step for material development to guide the direction for future research. When applied to hafnia, the EMRA illustrated that there are ways to mitigate most of the potential impacts (e.g., ecosystem destruction, use of fossil fuels, potentially unsafe working conditions and exposure to radioactive elements, land disputes, and supply concerns) associated with the material's known life cycle. The presented case study exemplifies the benefits of using the EMRA as a fast and cost-effective way to inform R&D decisions, as the positive risk assessment results suggest thin film hafnia as a sustainable potential replacement for relevant applications of PZT and encourage future research in the development of the material.

CRedit authorship contribution statement

Madison D. Horgan: Conceptualization, Methodology, Formal analysis, Investigation, Resources, Data curation, Writing – original draft, Visualization, Project administration. **H. Alex Hsain:** Conceptualization, Methodology, Formal analysis, Writing – review & editing, Supervision. **Jacob L. Jones:** Conceptualization, Methodology, Writing – review & editing, Supervision, Funding acquisition. **Khara D. Grieger:** Conceptualization, Methodology, Formal analysis, Writing – review & editing, Supervision, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.susmat.2022.e00524>.

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