Advances and challenges of Safe-and-Sustainable-by-Design: The case of high-entropy alloy coatings

Adamantia Kostapanou[1*], Spyridon Damilos[1], Evangelia Stamkopoulou[1], Konstantina-Roxani Chatzipanagiotou[1], Myrto Nikolakopoulou[1], Foteini Petrakli[1], Elias P. Koumoulos[1]

1. Introduction

In the last few years, the materials research community has seen a great increase in developing multicomponent alloys, known as high entropy alloys (HEAs) with extraordinary properties such as high-temperature and oxidation resistance and structural stability, allowing their use in structural and load-bearing components [1]. Notably, the global high-entropy alloy market size was USD 54.7 million in 2022 and the market is projected to reach USD 202.97 million by 2028, showcasing a compound annual growth rate (CAGR) of 24.42% during the forecast period [2]. The use of HEAs is beneficial in diverse applications in surface protection and engineering, due to their enhanced properties in various environments [3]. It is important to note that each HEA with minor elemental modifications is a new alloy base, therefore limitless combinations could be created [4]. Due to the novelty and the limitless variety of these materials, there is a gap between the research evolution on them and the occupational safety protocols that are required for their proper application. Additionally, the incorporation of sustainability in the design of HEAs not only takes into account the impacts of ores' extraction and metals' processing, but also it sheds light on the environmental concerns of alloys usage and their end-of-life options. The involvement of a large percentage of rare metals in the development of HEAs makes the consideration of sustainability aspects and possibly the inclusion of circular scenarios, imperative, aiming at resource efficiency, tackling the environmental impact of rare metals' mining and processing as well as the reduction of HEA manufacturing costs [5,6]. In order to examine the safety and sustainability level of these advanced materials, the newly developed five-step Safe-and-Sustainable-by-Design framework will be investigated, to support the design and development of safe and sustainable high-entropy alloys [7], as well as reviewing the applicability and limitations of SSbD methodology on the novel HEAs.

2. Framework and Methodology for Materials Safety & Sustainability

Safe-and-Sustainable-by-Design (SSbD) framework is applied as part of the EU funded M2DESCO project (Grant Agreement No. 101138397). M2DESCO is a collaborative, multidisciplinary research project aimed at developing next-generation high-entropy-

[1] IRES—Innovation in Research & Engineering Solutions, 1030, Schaerbeek, Belgium
[*] Corresponding author: Adamantia Kostapanou, mkostapanou@innovation-res.eu

alloy based multi-component green coatings (free of toxic substances) and sustainable (rare earth free & minimum critical metal elements) with predictable functionalities, performances, and life span. Through SSbD, the design criteria and requirements for the relevant coating materials and processes are assessed, while evaluating the models for the calculation of criticality and circularity values and for the selection and development of new coating high-entropy materials (HEMs) and processes (**Figure 1**). The methodology consists of two phases: i) the (re-)design phase that is applied at every stage of development (e.g., research, simulation, lab-scale, pilot-scale), using safety and sustainability design principles, defining the goal, scope and system boundaries of the assessment, and ii) the second phase, where SSbD assessment is applied at each gate or activity and scores feedback to the (re-)design phase, testing alterations to improve safety and sustainability. Reviewing the applicability of the SSbD framework on our case study, we investigate the selection of the materials and the design principles, such as material efficiency, minimization of hazardous chemicals usage, prevention of hazardous emissions etc., and assess the framework's suitability, gaps and limitations for novel advance materials. Within the first steps of the analysis, hazard assessment of the chemicals/materials to be used will take place, followed by the study of occupational risks during production and exposure of hazardous substances, and releases of the final product to the consumer and the environment. To make this possible we will review and employ all available information (e.g. the European Chemicals Agency (ECHA)) and investigate the applicability of ISO standards and publicly available online tools for risk assessment, developed for the chemical industry. In the later steps of SSbD methodology, environmental, social and economic aspects are being investigated based on available information and various tools. The goal is to perform a sustainability assessment that will demonstrate the overall impact of the chemicals and materials which are incorporated into the product's life-cycle.

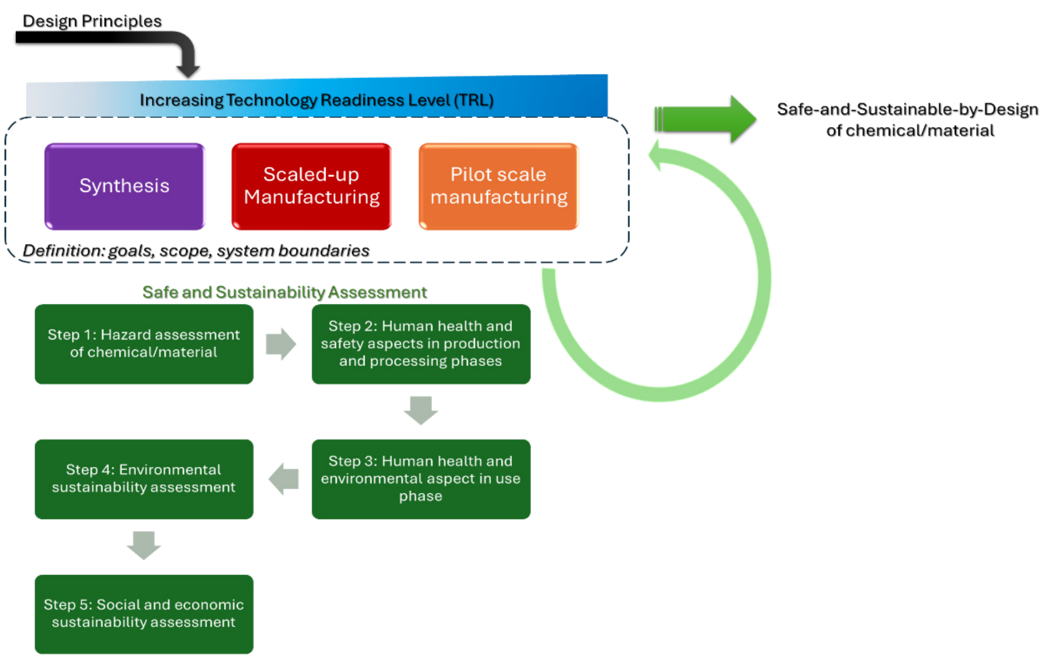

***Figure** 1. Integration of the SSbD framework in the project's innovation cycle.*

3. Conclusions

The outcomes of this study will provide a comprehensive evaluation of the applicability of the SSbD methodology to the production of novel HEMs and identify any gaps and limitations of the framework, while adding value to the concept of safety and sustainability to the materials industry.

4. Acknowledgements

Funded by the European Union under Grant Agreement No. 101138397. Views and opinions expressed are however those of the author(s) only and not necessarily reflect those of the European Union or HADEA. Neither the European Union nor HADEA can be held responsible for them.

5. References

1. Dewangan, S.K.; Mangish, A.; Kumar, S.; Sharma, A.; Ahn, B.; Kumar, V. A Review on High-Temperature Applicability: A Milestone for High Entropy Alloys. *Engineering Science and Technology, an International Journal* **2022**, *35*, 101211, doi:10.1016/j.jestch.2022.101211.
2. Business Research Insights High-Entropy Alloy Market Size | Global Report -2031 Available online: https://www.businessresearchinsights.com/market-reports/high-entropy-alloy-market-110243 (accessed on 29 March 2024).
3. Sharma, A. High Entropy Alloy Coatings and Technology. *Coatings* **2021**, *11*, 372, doi:10.3390/coatings11040372.
4. Krishna, S.A.; Noble, N.; Radhika, N.; Saleh, B. A Comprehensive Review on Advances in High Entropy Alloys: Fabrication and Surface Modification Methods, Properties, Applications, and Future Prospects. *Journal of Manufacturing Processes* **2024**, *109*, 583–606, doi:10.1016/j.jmapro.2023.12.039.
5. Nartita, R.; Ionita, D.; Demetrescu, I. Sustainable Coatings on Metallic Alloys as a Nowadays Challenge. *Sustainability* **2021**, *13*, 10217, doi:10.3390/su131810217.
6. Cann, J.L.; De Luca, A.; Dunand, D.C.; Dye, D.; Miracle, D.B.; Oh, H.S.; Olivetti, E.A.; Pollock, T.M.; Poole, W.J.; Yang, R.; et al. Sustainability through Alloy Design: Challenges and Opportunities. *Progress in Materials Science* **2021**, *117*, 100722, doi:10.1016/j.pmatsci.2020.100722.
7. European Commission. Joint Research Centre. *Safe and Sustainable by Design Chemicals and Materials: Framework for the Definition of Criteria and Evaluation Procedure for Chemicals and Materials.*; Publications Office: LU, 2022.