Bridging AI and Sustainability: Advancing Safe and Sustainable by Design (SSbD) for Next-Gen Coating Materials

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Key Words: ***Life Cycle Assessment (LCA), Safe and Sustainable by Design (SSbD), sustainability, Predictive tool, Green Transition, Data-driven Sustainability.***

Abstract

High entropy alloys (HEAs) are an emerging materials category of advanced materials (AdMas) that gained attention not only for their superior mechanical and chemical properties, very promising for coatings production (high entropy coatings-HECs), but also for their sustainability performance throughout their entire lifecycle. The newly introduced by the European Union (EU) Safe-and-Sustainable-by-Design (SSbD) [1] framework for chemicals and materials was designed to stir the innovation process from early stages towards safer and greener materials. This holistic approach incorporates different sustainability aspects (safety, environmental and socio-economic) and also identifies hotspots at low technology readiness level (TRL) facilitating the procedure of green transition on materials sector. Furthermore, machine learning (ML) tools have gained significant interest from the scientific community, as incorporating them will aid the efforts for sustainable alternative materials development in various fields, including HEAs and HECs. Harvesting the full potential of such tools will not only enable the discovery of relationships within datasets more efficiently, but it will also facilitate decision-making at all TRLs by identifying patterns and predictiveness of material properties.

To ensure that HEA coatings are designed efficiently, safely, and with minimal environmental impact from the very beginning, an integrated workflow will be implemented that combines molecular dynamics modelling for HEAs and coating process modelling (PVD) with SSbD criteria, risk and safety evaluation, and sustainability predictions. Within this framework, IRES will develop an ANN-based predictive tool for sustainability, bridging the gap between experimentation and LCA and addressing the challenge of data scarcity in early-stage material design. The model will generate high-quality, low-uncertainty life cycle inventory (LCI) data to be utilized for life cycle modelling. This tool will provide real-time sustainability impact assessments, providing LCIA results to support SSbD evaluations, identifying hotspots and ensuring early-stage safety, environmental and economic predictions during material design. The approach will also include a thorough evaluation of end-of-life scenarios, integrating the 6R Strategies of Circular Economy, as well as indicators related to circularity and use of critical metal elements. The outcome of this study will provide an advanced approach through data generation and contribute to the research community as a decision-making tool for effective implementation of the SSbD methodology towards next-generation, green coating materials. All in all, by integrating AI-driven predictions with SSbD methodologies, this approach advances next-generation coating materials that align with EU sustainability goals, offering a robust decision-making framework for researchers and industry stakeholders.

Acknowledgements

The authors acknowledge the M2DESCO project, 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.

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