Computational Multi-Models Enabled Design of Safe & Sustainable Multi-Component High-Entropy Coatings – M2DESCO

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Abstract

M2DESCO - HORIZON-CL4-2023-RESILIENCE-01 is a collaborative, multidisciplinary research project aimed at developing next-generation high-entropy-alloy (HEA) 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. The purpose of the project is to increase wear resistance by 100%, corrosion/oxidation resistance by 50~60%, of metal components, while effectively reducing the criticality of coating materials by at least 70%.

To achieve these goals, the project shall to integrate AI/ML underpinned, highly effective and highly efficient Computational Modelling that is guided by a novel Safe and Sustainability by Design (SSbD) framework and facilitated by high-throughput characterisations and evaluations, to speed up material-design and coating-product development process (reducing the development cycle-time by 400~500%), and concomitantly the overall product manufacturing cost by 20% due to use of the new tooling developed.

For example, the properties prediction of the new HEA coating materials is carried out combining and interconnecting physical models, from first principle atomistic (density functional theory, and molecular dynamics) to continuum mechanistic modells, including the development of non-equilibrium kinetics based synthetic routes. The interconnectivity of all the models applied requires a rigorous data management structure, so based on the current MODA Standards.

High throughput experimental production, from sample production to fundamental characterizations shall support the robustness of the physical models developed. In particular, two families of HEA coating materials are the focus of the M2DESCO research. The group 1 consists of equimolar AlTiCrMoW nitride coatings, with promising applications in tooling surface protection (cutting and forming tools). The group 2 relies of the developed CrCoNi-FeMn[1] coatings with outstanding combinations of strength and toughness, and large potential to exhibit notable corrosion protection.

[1] Dong Liu et al. ,Exceptional fracture toughness of CrCoNi-based medium- and high-entropy alloys at 20 kelvin.Science378,978-983(2022).DOI:10.1126/science.abp8070

M2DESCO intends to adopt the SSbD framework[2] through integration of the associated criteria into enabling tools, for the development of SSbD HEA coating materials and production processes. The methodology is to be implemented along the innovation process at every stage in the value chain of HEA coatings' development and consists of five steps, including hazard assessment, human health and safety, environmental safety, environmental sustainability, and socio-economic sustainability, along the product's entire lifecycle.

The advances of M2DESCO will contribute significantly to combating the loss in EU region caused by corrosion and wear, to the enhancement of the global profile and leadership of the EU material modelling/research community, to strengthening of the innovation capability of the EU coating industry/business, and ultimately to reinforce the PVD EU sector which leads a world-wide market projected to reach 40.97 billion in 2028, thus, rendering great benefit to the wider advanced manufacturing chain, and effectively enhancement of the global competitiveness and the resilience of the EU industry.

[2] https://publications.jrc.ec.europa.eu/repository/handle/JRC128591