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

Gonzalo García Fuentes[1], Yi Qin[2], Hanshan Dong[3]

1. Introduction

M2DESCO - HORIZON-CL4-2023-RESILIENCE-01 [1] is a collaborative, multidisciplinary research project aimed at developing next-generation high-entropy-alloy based multicomponent 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%. The project counts on the participation of AIN as coordinator, the Universities of Strathclyde (UK) and Birmingham (UK), the Politecnico di Torino (IT), the National Technical University of Athens (HE), the National Research & Development Institute for Non-ferrous and Rare Metals (RO) and the SMEs: Anter Ltd (HE), Durante Space Tech (ES), PVT GmbH (D), Innovation in Research & Engineering Solutions (BE), Laneko S.A.L. (ES) and Innovative Coating Solutions (BE).

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 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.

The advancement 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.

The project will spin around the knowledge enhancement of 5 different THEMEs, as depicted schematically in Figure 1:

[1] Asociación de la Industria Navarra, 31191 Cordovilla (Navarra, Spain) email: gfuentes@ain.es
[2] Dpt. Design, Manufacturing and Engineering Management. University of Strathclyde Glasgow
[3] School of Metallurgy and Materials. University of Birmingham

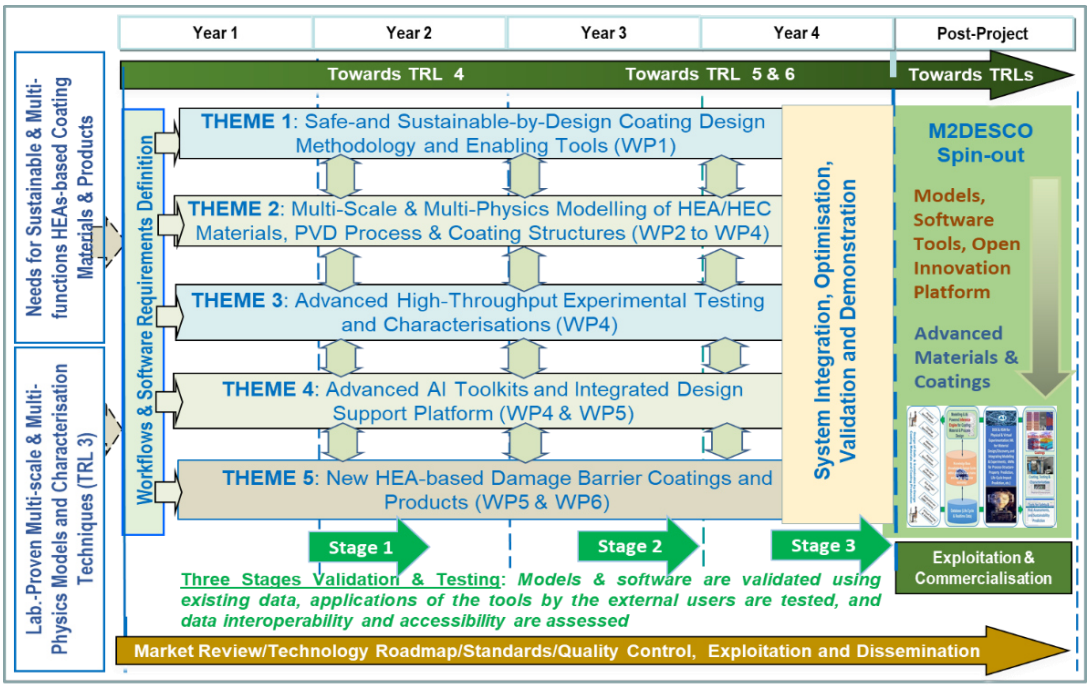

Figure 1: M2DESCO project development pipeline

(i) Safe-and Sustainable-by-Design Coating Design Methodology and Enabling Tools. This topic intends to adopt a "Seven-Steps Approach" for SSbD coating materials and production processes and includes the development of Combinatorial Safety and Risk Assessment (SRA), and Hybrid Life-Cycle Assessment and prediction.

(ii) Modelling of the Coating Processes and Film Growths encompasses the calculation of phase diagrams and thermodynamics of HEA configurations for low criticality combinations of coating materials. It will make use of Density functional theory (DFT), molecular dynamics (MD) and finite element (FE) cohesive-zone calculations, all interacting at different atomic-cluster-continuum scales. Theme 2 also includes calculations of coating processes and film growth by the development of kinetic Monte-Carlo non-equilibrium approaches. This topic is framed in a multiscale model framework, so the models and approaches cover different dimensional range of the materials and microstructures (from atomistic to macroscopic scale) and connect each other through well-defined input-output model parameters.

(iii) Advanced High-Throughput Experimental Testing and Characterisations will permit to accelerate the obtention of reliable datasets to aid the construction of predictive models and implement feedings to AI-tools.

(iv) Advanced AI Toolkits and Integrated Design Support Platform shall be constructed to integrate the above model functions and apply AI tools in an effective manner.

(v) New HEA-based Damage Barrier SSbD Coatings and Products will be produced experimentally on selected use cases: (a) hot forging and (b) machining of difficult to cut metals, both in order to quantify the benefits of the developed coatings and the lowering of the materials/processing environmental and economic impacts. References

[1] M2DESCO contract nr 101138397. web-link at the Horizon Europe site.