

Recent progress in Integrated Computational Materials Engineering (ICME) development of novel coating materials: the CoBRAIN project

Giovanni Bolelli

Department of Engineering "Enzo Ferrari", University of Modena and Reggio Emilia, Modena, Italy

This presentation provides an overview of the “CoBRAIN” project (proj. n. 101092211, HORIZON-CL4-2022-RESILIENCE-01-19) and its results. CoBRAIN seeks to devise sustainable alternatives to conventional wear- and corrosion-resistant materials by exploring the vast compositional space of High-Entropy Alloys (HEAs), but, more in general, it seeks to establish an integrated approach to the design and selection of coating materials. Thus, rather than relying on few materials with a “one size fits all” approach, CoBRAIN is establishing tools and methodologies for the rapid identification, validation and production of novel materials adapted to the specific requirement of each application.

In the CoBRAIN project, we established an integrated computational workflow where various high-throughput physical modelling techniques generated a large amount of complementary data on HEA properties and features as a function of their chemical composition. We therefore obtained datasets on equilibrium phase composition, stacking-fault energy (a predictor of the main deformation mechanism of a metallic material under applied strains), microstructural evolutions during high-rate solidification, and micromechanical properties. In parallel, a high-throughput experimental workflow was also set up to test and validate coating solutions based on HEAs and on TiC-HEA cermets. The workflow includes feedstock materials production in powder form through mechanical alloying; coating deposition by thermal spraying techniques (HVOF, HVAF, cold gas spray); and microstructural, mechanical, and functional characterization of the resulting coated samples. A machine learning API was then developed by training neural network-based models on the experimentally validated datasets, integrated with literature data where needed. A Sustainable Decision Support System (SDSS) interface is being created, which integrates the ML API to generate candidate HEA compositions based on input specifications; a Life Cycle Performance Analysis (LCPA) tool to verify the sustainability of the solutions, both from the economical and the health, safety and environmental points of view; and the experimental knowledge base itself for additional data.