HORIZON-CL4-2022-RESILIENCE-01-19

AiMPACT

ADVANCED MATERIALS MODELLING & CHARACTERISATION CLUSTER

DATA

- Development of common methodologies for data processing.

DATA SHARING & STORAGE

- Procedures for AI-based image analysis.
- Sharing SEM and TEM images for training ML tools.
- FAIR data repositories.

AI-DRIVEN TOOLS

Advanced high-strength steels are essential for the EU's strategic sectors, including Renewables, Space&Defence, E-mobility, and Energy. Reducing greenhouse gas emissions requires new materials and scalable manufacturing methods. However, the EU steel industry depends on imported alloying elements, facing supply risks and rising costs.

Backed by a 10 European partners, AID4GREENEST develops AI-driven characterisation methods and modelling tools for steel design, process optimisation, and performance assessment to enhance material quality, cut emissions, reduce waste, and mitigate supply chain vulnerabilities for critical raw materials.

Three AI-driven tools are in development, as well as a machine-learning model to predict creep performance, a sequential model to simulate microstructure evolution in forging and quenching, and an AI-powered platform for knowledge sharing and standardisation.

ML-BOOSTED MATERIALS DISCOVERY

The project will demonstrate a science-based approach to the development of electrode materials forming key parts of reversible chemical-to-power cells. Such devices can operate in two modes: in fuel cell (FC) mode, it converts hydrogen into electricity whereas when operating as electrolyser cell (EC), it uses excess electricity to form hydrogen from water electrolysis. This versatility enables the integration of intermittent renewable energy sources with the electrical grid by storing the excess energy as carbon-free chemical fuel. In particular, the project targets mixed oxides with perovskite structure with minimised critical content while keeping highest possible performances and targeting fair economic viability.

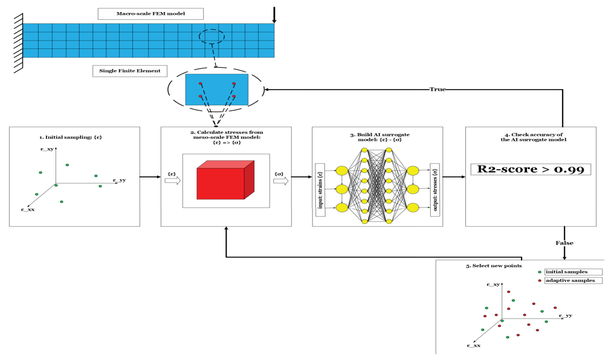
In particular, the project integrates a smart combination of advanced technologies, involving tailor-made materials preparation, harmonised and ground-breaking characterisation methods, multi-scale modelling and AI-enabled tools. This corpus of open-minded, innovative, reliable, and use-relevant methodologies targets the discovery of the scientific knowledge required to sustain the rational design of optimized candidate electrode materials.

- Enable a model-based innovation processes covering all stages from materials design to product development, including validation, characterisation and life cycle assessment.
- Contribute to border-crossing harmonised methodologies for materials discovery.

AI-SURROGATE MODELLING

Multiscale analysis of structures is computationally costly. Therefore, surrogate modelling techniques using artificial intelligence are widely used to reduce the cost without any loss in terms of accuracy composite.

Our method combines an adaptive sampling methodology to develop an active learning strategy that can explore and exploit the input space and select the most informative missing points to build the surrogate model.



Our main goal is to incorporate the above procedure in finite element packages that examine the multiscale behavior of composite structures in fatigue and fracture for the aerospace, car manufacturing and wind energy turbines industries.

KEY INNOVATION

- Novel X-ray and electron-probe based characterisation workflows and protocols for power semiconductor materials.
- Modelling concepts for better characterisation and lifetime prediction of power semiconductor interconnect materials.
- Establish FAIR and open data practices to enable efficient data workflows between characterisation and modelling techniques.

CHADA - MODA - EMMO

- **Development of common ontologies domain in collaboration with EMMC and EMCC.**
- **Exchange architectures and best practises for ontologies and workflows.**

OPEN DATA AND INDUSTRY-DRIVEN ENVIRONMENT FOR MULTIPHASE & MULTISCALE MATERIALS CHARACTERISATION & MODELLING COMBINING PHYSICS AND DATA-BASED APPROACHES

MatCHMaker INNOVATION CASES

Construction: Decrease CO2 emission and waste of cement production; *maximum substitution of clinker while maintaining equal/superior performance*.

Energy: Solid Oxide Fuel/Electrolysis Cells; *produce hydrogen without CO2 emissions and achieve the highest efficiency.*

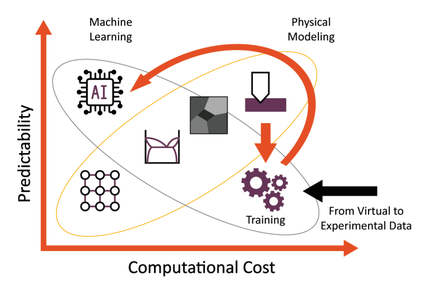
Mobility: Proton-Exchange Memberane Fuel Cells; *Produce zero-emission power in multiple applications.*

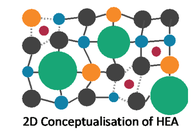
OBJECTIVES

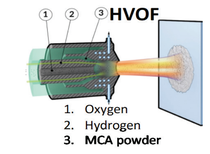
- to accelerate advanced materials development.
- enhance traceability, integrity and interoperability of data.
- create an open data repository manufacturing processes.

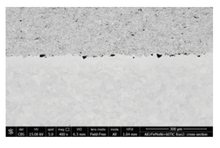
SUSTAINABLE COATING MATERIALS

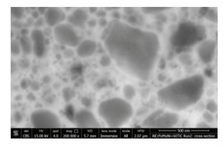
Protective coatings are increasingly needed to improve the performance and efficiency of industrial processes. However, existing coating solutions like WC-Co or electroplated chromium rely on toxic and/or critical materials, thus posing environmental and economic sustainability issues.











High-entropy hardmetals (HHM), consisting of a high-entropy alloy (HEA) matrix with hard-phase reinforcement, are a novel category of materials with considerable potential as sustainable coating solutions. The CoBRAIN project integrates physical modelling, artificial intelligence and advanced characterization for high-throughput exploration of the vast compositional space of HEAs/HHMs to devise optimal, sustainable coating solutions.

EC/HaDEA is supporting six running projects investigating a relevant range of characterisation methods, models and simulation tools to enhance the design and development stages of advanced materials and products, focusing on user cases related to **low carbon and clean industry applications.**

AddMorePower	aid4 GREENEST	CoBRAIN	standart	KNOWSKITE-X	MatCHMaker
Advanced modelling & characterisation for power semiconductor materials & technologies	AI Powered Characterisation & Modelling for Green Steel Technology	Integrated Computational / Experimental Material Engineering of Thermal Spray Coatings	Durability Modelling of Composite Structures	Knowledge-driven fine-tuning of perovskite-based electrode materials for reversible Chemicals-to-Power devices	Advanced Materials Characterisation & Modelling
GA No 101091621	GA No 101091912	GA No 101092211	GA No 101091409	GA No 101091534	GA No 101091687

JOINT STRATEGY

- **Common research timeline** with regular cross-fertilisation and updates.
- **Common aim** for an intense research exchange and joint dissemination activities throughout their whole duration bringing together research from different disciplines.
- **Common research topics of interest:** LCA studies, stakeholder consultation, multiscale material modelling and characterisation, integration of modelling and characterisation, AI-driven tools, advanced materials, high-throughput materials design.
- **Contribution to standardisation:** DST, CoBRAIN and MatchMaker participated to the revision of CWA 17815:2021 (CEN-CENELEC).
- **Add Match maker:** advances in characterisation methods.

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