About the project

The EU-funded ICARUS-SW project introduces a mathematical tool able to describe the thermodynamics of polycrystalline materials. ICARUS-SW is a software tool that can be applied on materials where surfaces are of prime importance, like coatings, thin films and catalysts.

As a step forward, an underlying innovative idea of the project is to use the ICARUS-SW software as a predictive tool for the exploration, identification and design of new thermodynamically stable multi-component nanocrystalline (nc) metal alloys with enhanced thermal, mechanical and irradiation damage self-healing properties.

ICARUS-SW software allows the systematic exploration of the parameter space defined by chemical composition, microstructure, thermodynamic state functions and properties in search of new families of nc alloys. In preparation of this software, the exploitation, IPR and dissemination strategies will be defined and implemented in this project, based on in-depth market analysis, business planning and other exploitation related activities.

The project is funded under the EU Framework Programme for Research and Innovation (Horizon H2020) as a FET Innovation Launchpad action. The overall objective of the project is to support the research result of the linked FET ICARUS Project (theoretical model) evolve from TRL3 to a commercial and social innovation (final software) by involving potential users and other relevant stakeholders, understanding the market environment and outlining potential exploitation paths.

The Team

BRIMATECH

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ICCRAM International Research Center in Critical RAw Materials for Advanced Industrial Technologies

easn Technology Innovation Services

Start Date: May 1st, 2019
Duration: 12 months
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Scan & visit ICARUS-SW website

Design by EASN-TIS

ICARUS SW

ICARUS-SW

Ambitious steps towards the first software that describes & analyses the grain boundary of materials

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 851644

Innovation Idea

The status

There are several commercial Calphad software products on the market for the simulation & modeling of phase diagrams and thermochemistry supporting the exploration of new materials. Yet up to now, they are not taking into consideration the grain boundaries.

The concept

ICARUS-SW software not only considers but also enables the description of the grain boundaries. Moreover, it offers nano-specific calculations (NanoCalphad) as well as the possibility of describing the nanostructure of materials. Thus, specific alloys for surface applications can be designed and new nc alloys can be identified and predicted. For the thermodynamic modeling, a statistical mechanical approach is used where thermodynamic state functions and auxiliary quantities are described mathematically in terms of chemical composition and atomic species distribution in both crystalline grains and intergranular disordered interfaces. The theoretical models were developed & tested in the frame of the linked FET ICARUS Project and provide scientifically proven & validated algorithms for later software development, enabling the design of new generation alloys.

The Software

Key Features

Pre-screening of potential thermodynamically stable nc alloys.

- Selecting the most optimal alloying elements in order to obtain thermal stability in the resulting material.
- Indicating the particular elements proportion which gives the alloy thermal stability.
- Enabling the user to select the desired grain-size.
- Providing the processing temperature and service temperature of the alloy.

The model has currently application to binary metallic systems while there is the possibility to be expanded to ternary and quaternary systems.

Application Areas

Conceptually new structural materials, engineered nanostructures for catalysis & energy production, radiation-tolerant metals, lightweight alloys, corrosion-resistant coatings/thin films will become available unlocking many challenges faced nowadays by science and technology in the various fields.

ICARUS-SW intends to improve

30% time to market

20% development costs

Impact

New families of materials with unprecedented properties and performances

The resulting software enables the material research, development & design community to more quickly explore, identify and design new thermodynamically stable multi-component nc metal alloys with enhanced properties.

A tool that significantly reduces product development time and costs

A new alloy requires a high amount of experiments the ICARUS-SW tool can decrease these experimental trials as it focuses on the most promising combinations of elements.

Substitution of Critical Raw Materials (CRMs)

Novel alloy development becomes less complex or challenging. This will help a company, sector or economy to reduce its reliance on imported CRMs. Society will benefit from an improved path to innovations across the related industries and increased competitiveness of the European materials industry, mitigating the external dependence.

Maintaining European competitiveness with leading developments

The project contributes to the focus on new engineered materials in the European Research Agenda and helps European stakeholders increase competitiveness industry, mitigating the external dependence.