Computational Multi-Models Enabled Design of Safe & Sustainable Multi-component HEA

M2DESCO

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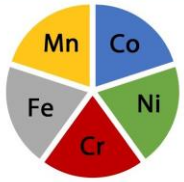
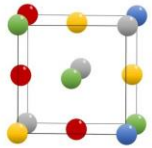
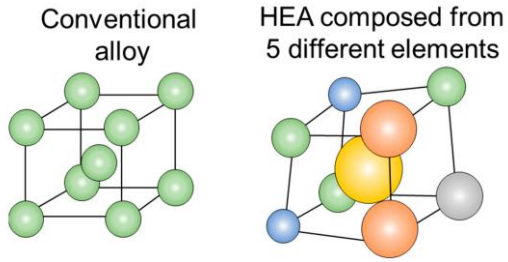
WHAT & WHY HEA Coatings

High entropy alloys





$$\Delta S_{conf} = -R \sum_{i=1}^{n} x_i \ln(x_i)$$



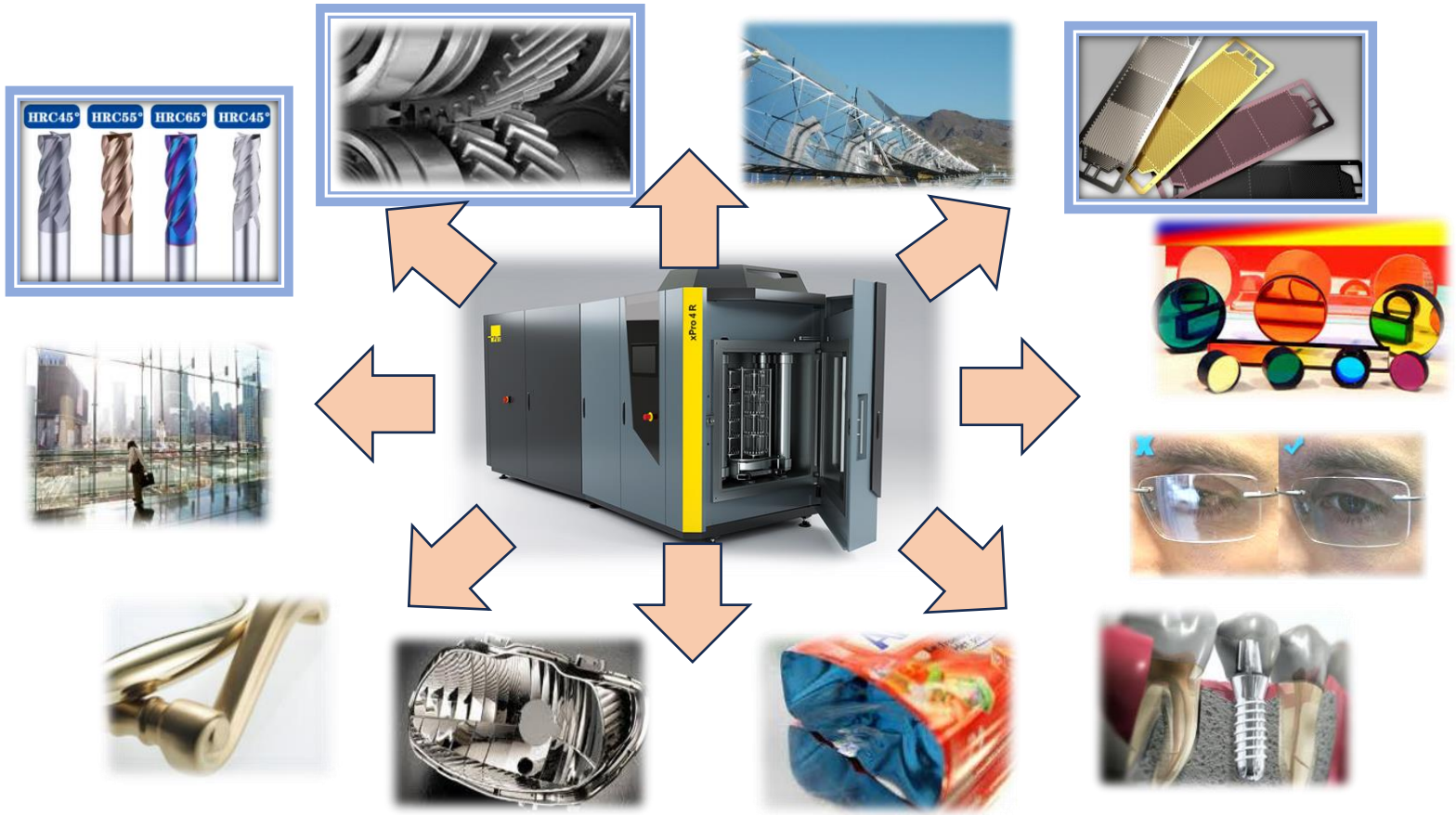
Enhanced mechanical strength by solid solution hardening

Enhanced thermal and chemical stability due to sluggish diffusion

Enhanced fatigue/wear resistance in harashing environments

A multi-element alloy formed by 4 or more constituents, yielding a (non-equilibrium) solid solution. It can be equimolar to maximize the mixing term of the conf. Entropy.

The Physical Vapour Deposition: a high tech business EU is leading



B2B

or

B2C

Physical Vapour Deposition is a key enabling technology to produce thin films of tailor properties. It encounters numerous applications, tooling, optics, energy,…..

Recent interest in HEAs prepared in the form of thin film by PVD-sputtering

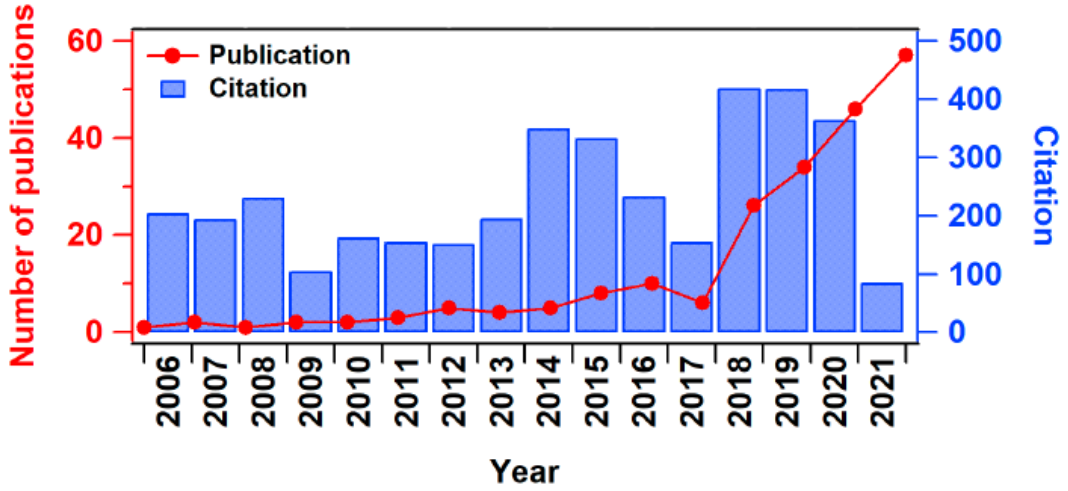
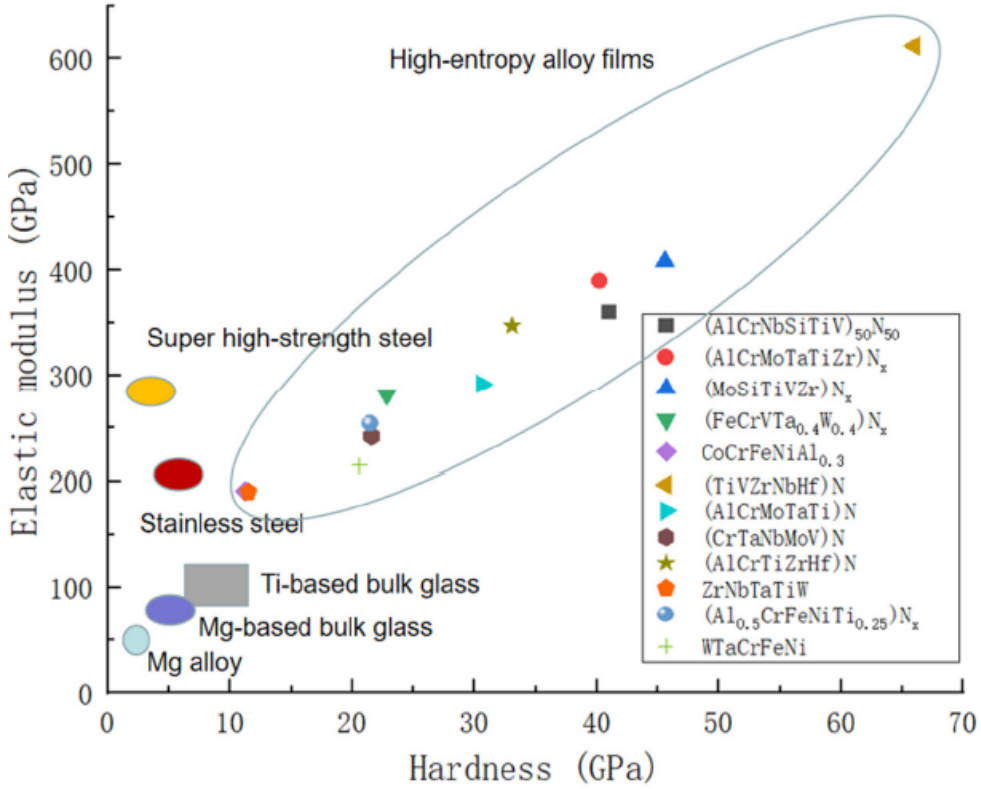


Figure 1. Number of reported publications on magnetron-sputtered HEFs. The histogram shows the number of the articles from 2006 to December 2021. The red curve displays the citation number of the articles per year. The results are plotted according to statistical analysis from the Scopus website.

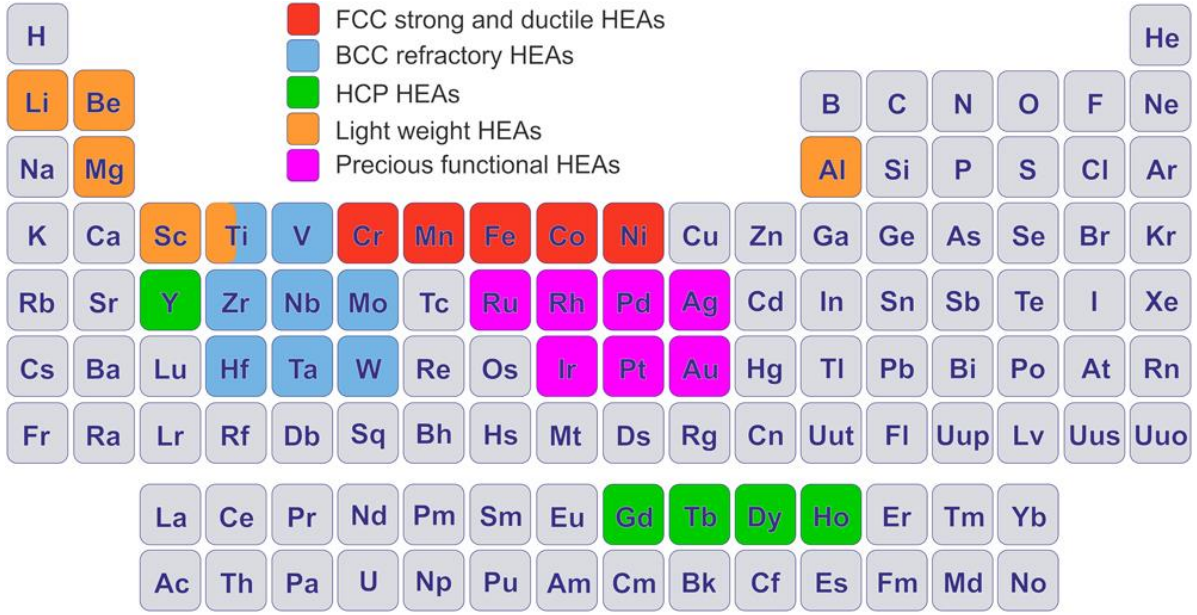


High-Entropy Alloy Films. Coatings **2023**, 13, 635

CHALLENGES WHEN DESIGNING HEA COATINGS, …., WHICH COMBO SHALL I USE?

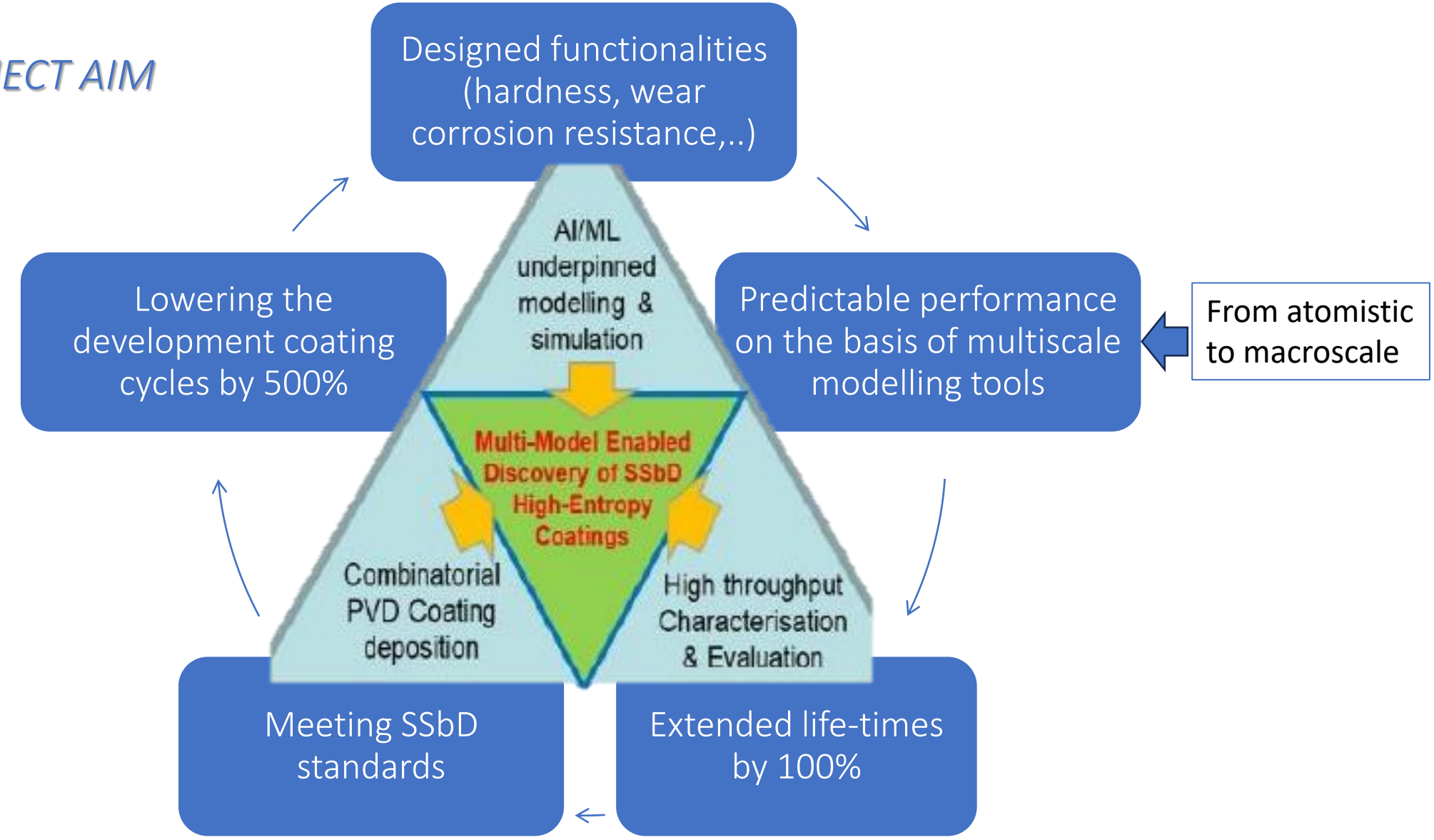
High degree of freedom in alloy design → combinations of 64 potential elements → 10^8 combos!!

Development of coatings (incl. HEAs) based on trial-error. Unaffordable to make wide explorations

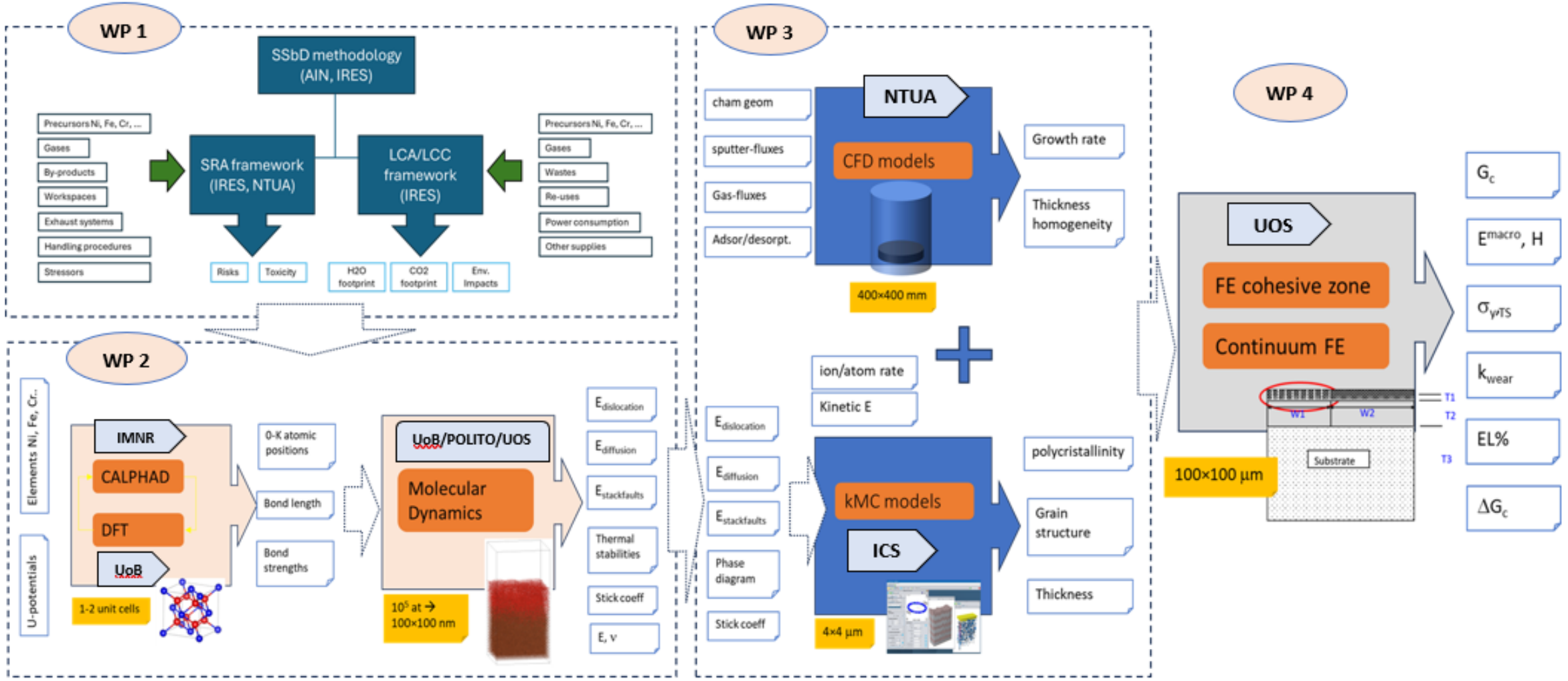


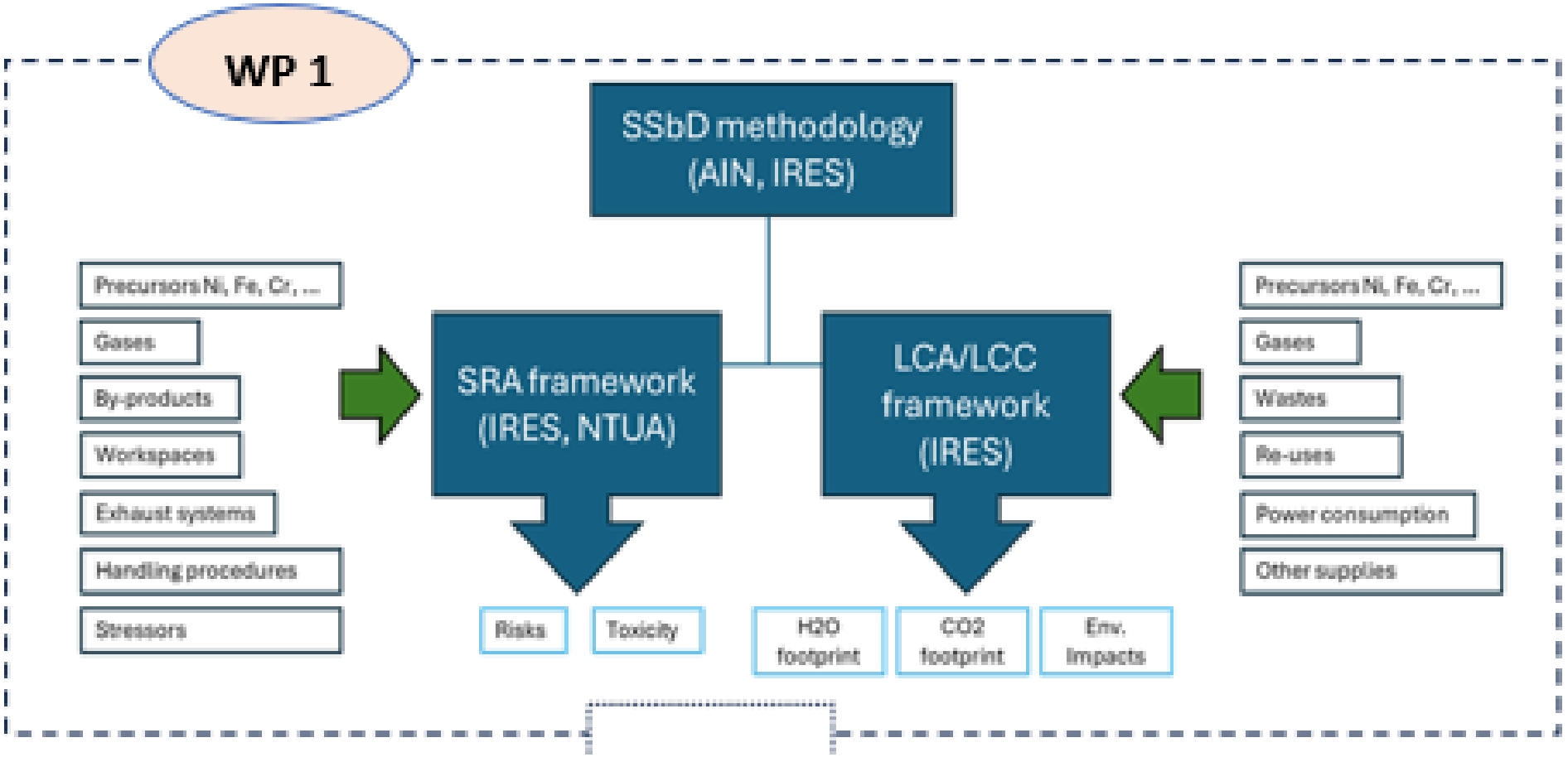
Warning!! - increased use of critical metal elements (such as Nb, Co, V, W) or hazards (VI-Cr)

M2DESCO PROJECT AIM

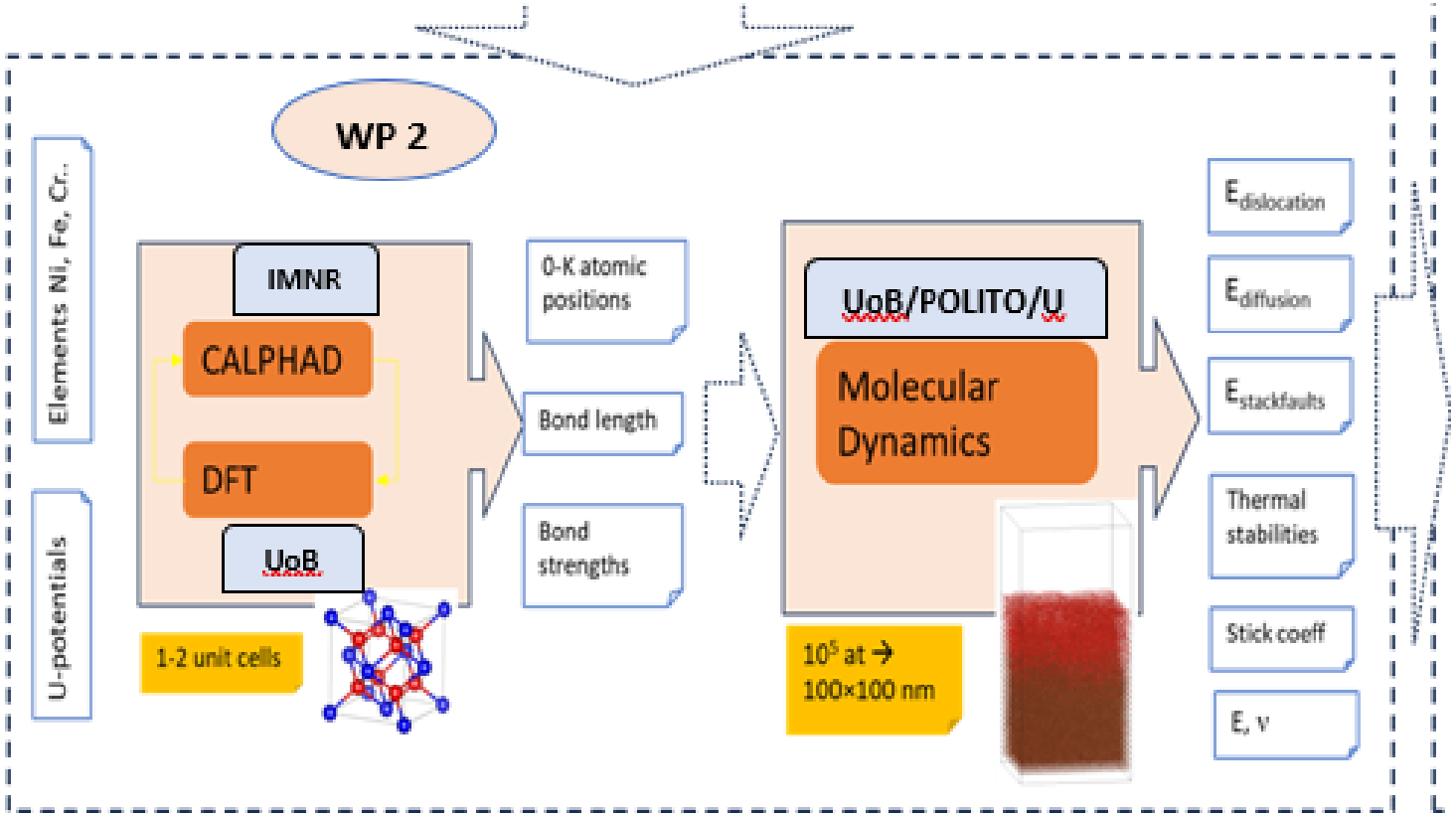


THE MULTISCALE MODEL – How to interact betwen size scales



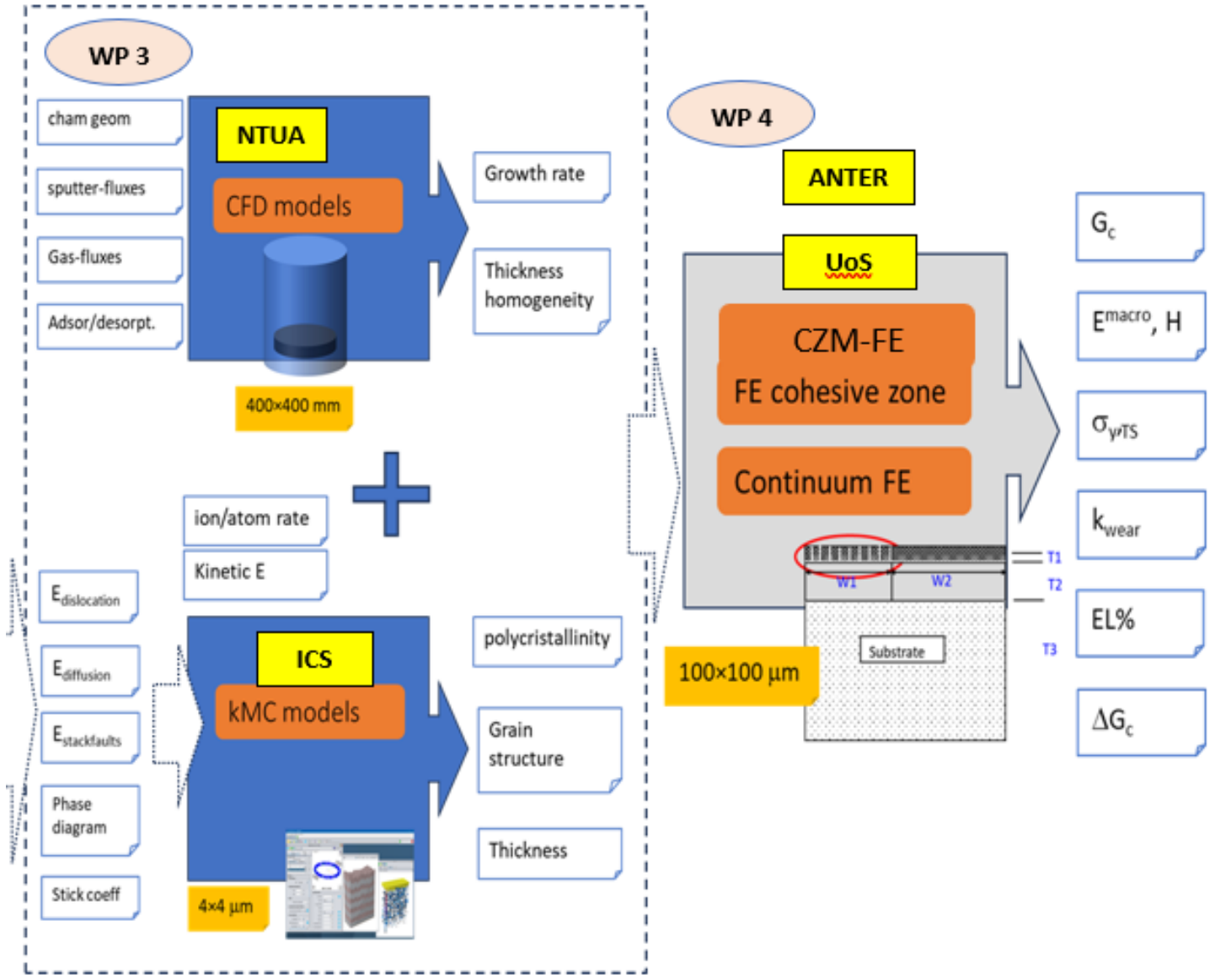

WP 1
SSbD methodology (AIN, IRES)
SRA framework (IRES, NTUA)
LCA/LCC framework (IRES)
Precursors Ni, Fe, Cr, ...
Gases
By-products
Workspaces
Exhaust systems
Handling procedures
Stressors
Risks
Toxicity
H2O footprint
CO2 footprint
Env. Impacts
Precursors Ni, Fe, Cr, ...
Gases
Wastes
Re-uses
Power consumption
Other supplies

Inputs from WP1, selection of non toxic species



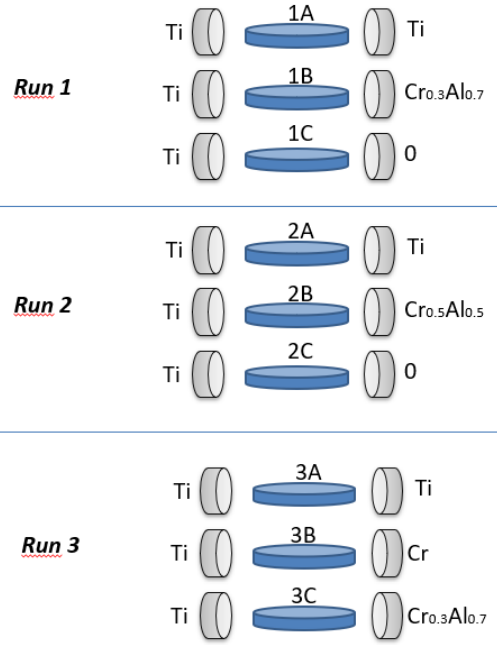
outputs to meso and microscales

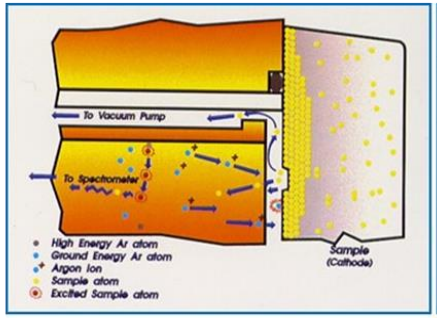
Inputs from atomic & molecular scales



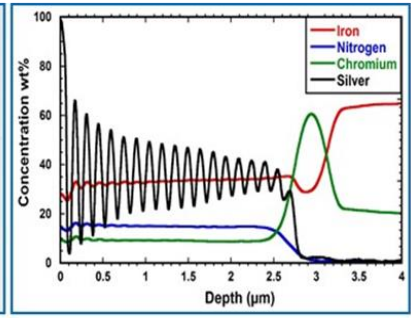
High Throughput (HTP) experimental production

Setup



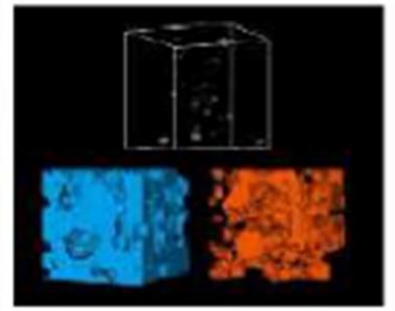


(a) GDOES



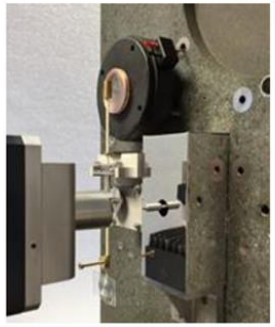
(b) Composition depth profiles

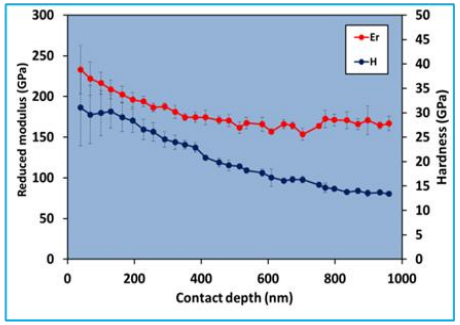
(a) Robomet 3D



(b) 3D microstructural

XRD Phase identification





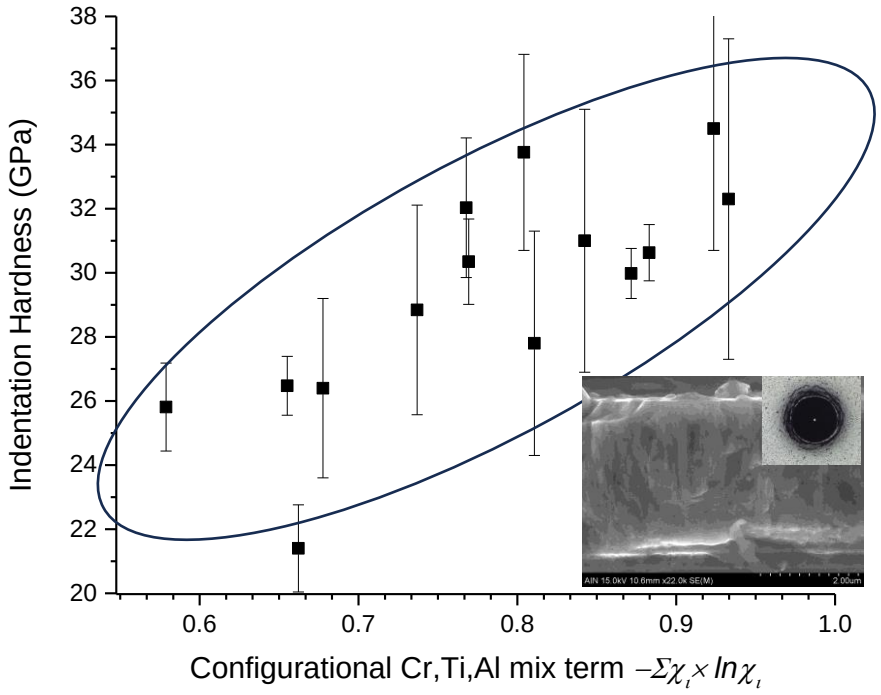
Nanoindentation
Dynamic Mechanical Compliance testing (DMCT)

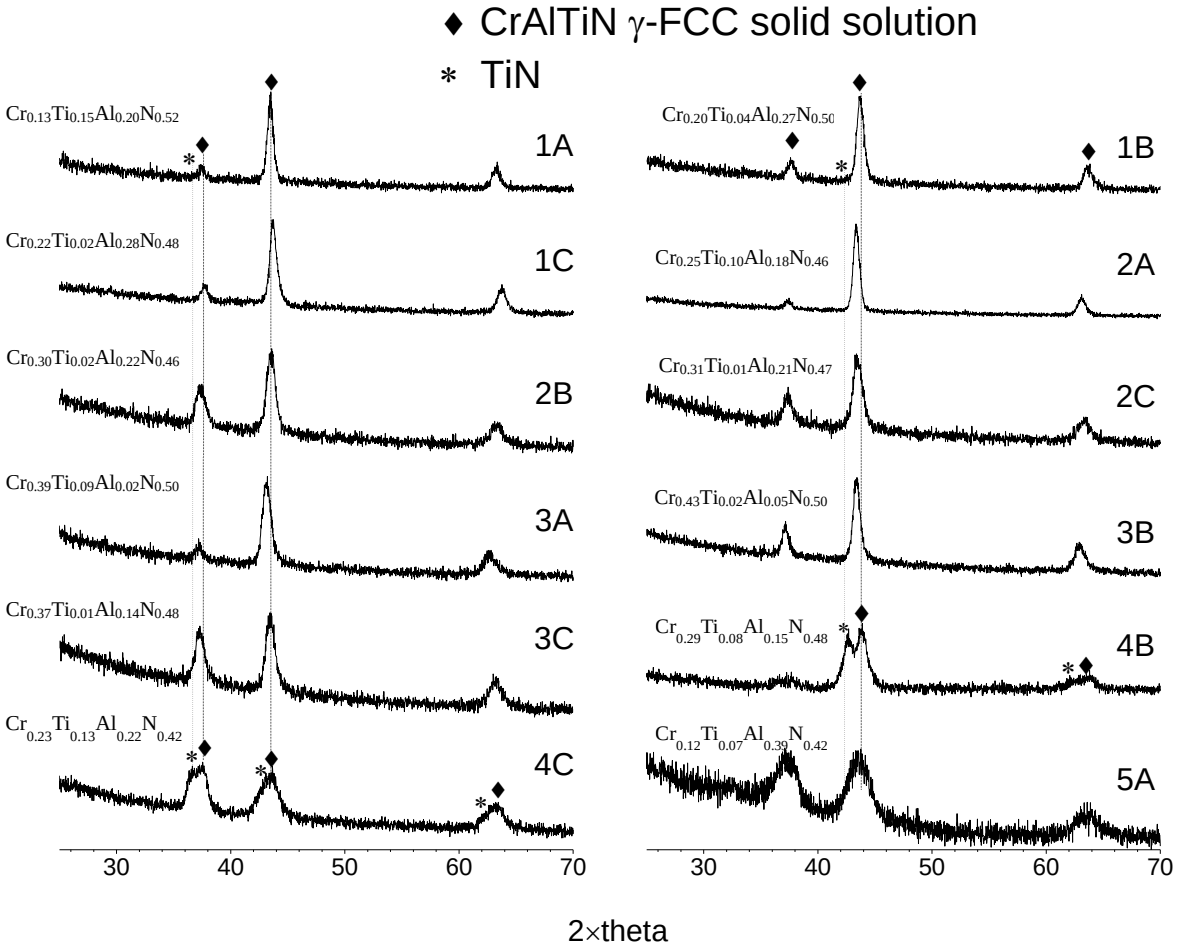
Multitarget PVD coating production

Fast analytical techniques

Previous experimental results

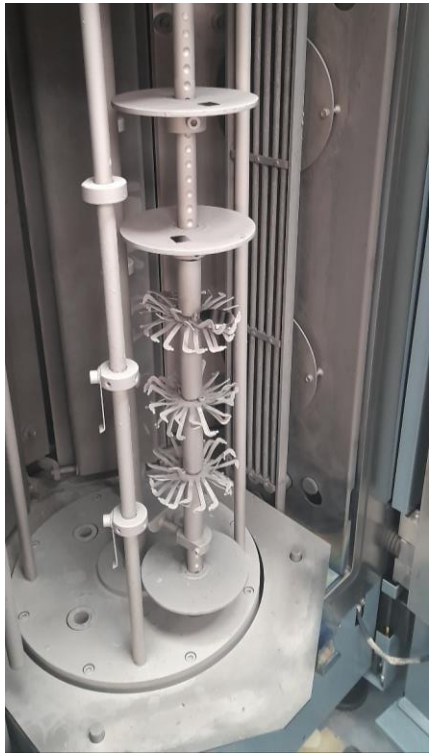
First experimental evidence of interdependencies between config entropy term and indentation hardness





GG. Fuentes et al Surface & Coatings Technology 420 (2021) 127326

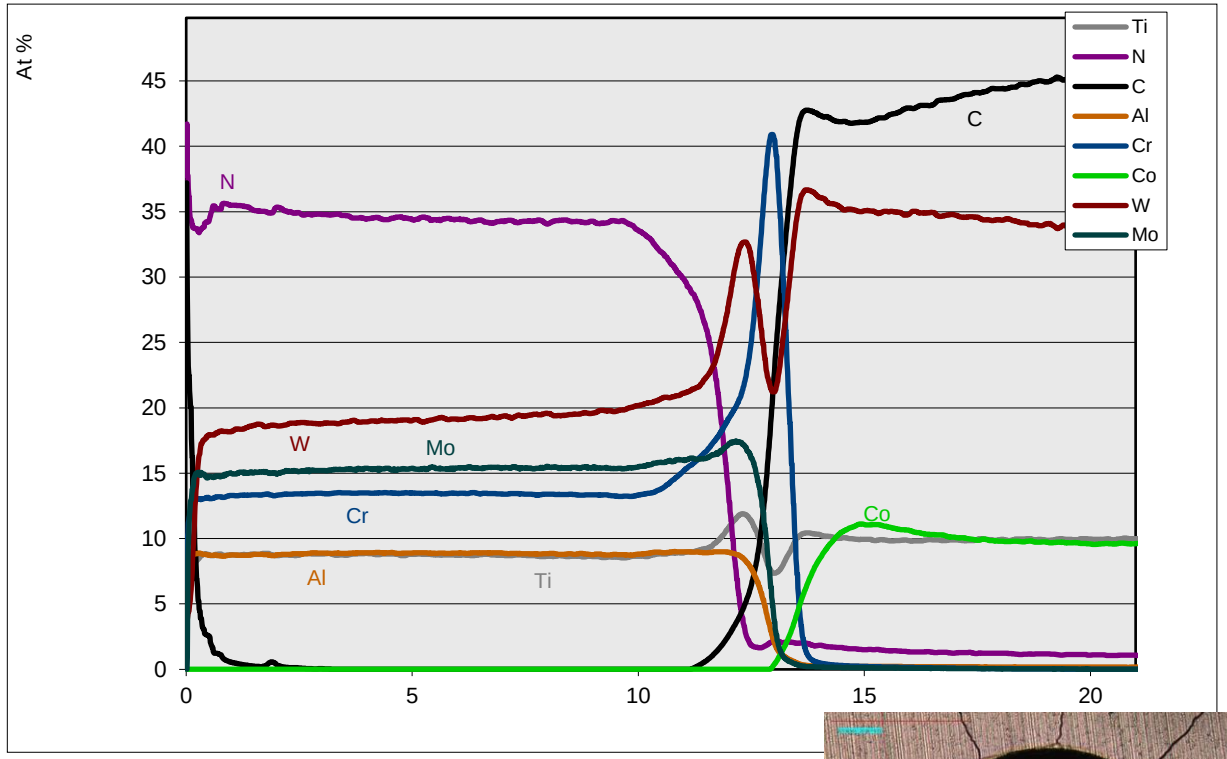
FIRST EXPERIMENTAL DATA ON HEA coatings

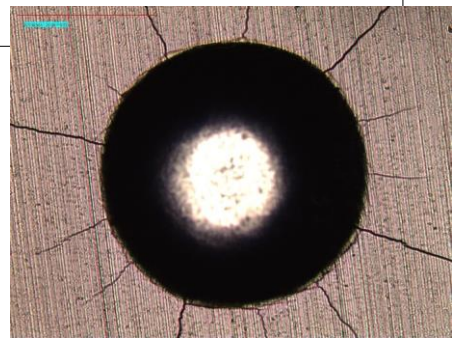


Plasma Vakuum Technik GmbH
https://www.pvtvacuum.de/

- Magnetron sputtering DC_pulsed
- Target AlTiCrMoW equimolar
- N2 gas Flow (studied as parameter)
- Substrates WC-Co (for machining tools)
- Tests:
  - GDOES (composition)
  - Calotests (thickness)
  - Wear

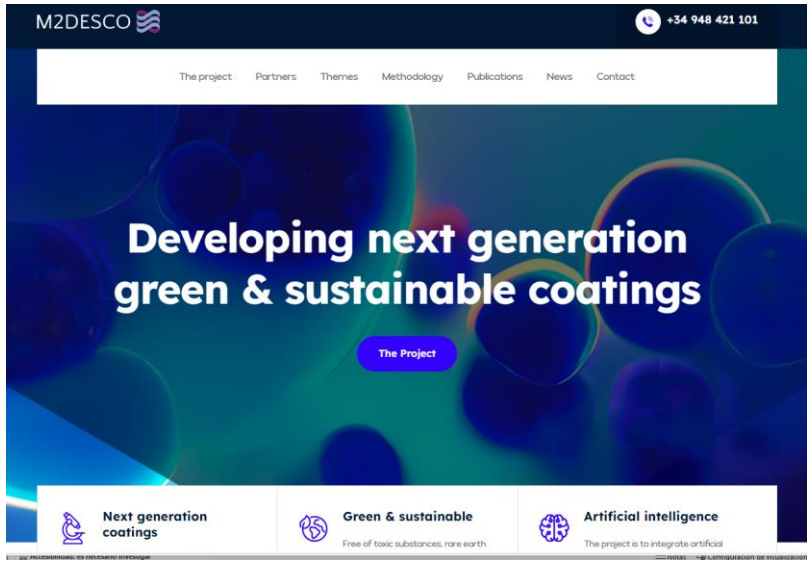
FIRST EXPERIMENTAL DATA ON HEA coatings





- Equimolar target sputtering leads to non-equimolar coating compositions. The larger the mass the bigger the wt% in the coating (transport effects?).
- Excellent adhesion strength.
- So far, good wear behaviour against 100Cr6 in friction tests.
- Pending analyses
  - Crystal and micro structures
  - Hardness
  - Additional wear tests (T, load, etc)

MORE DETAILS NEXT

Keep updated (outcomes, news) at:

https://m2desco.ain.es/demo/