Prediction of the strength of Fe-Ni-Cr-Co high entropy alloy single crystals

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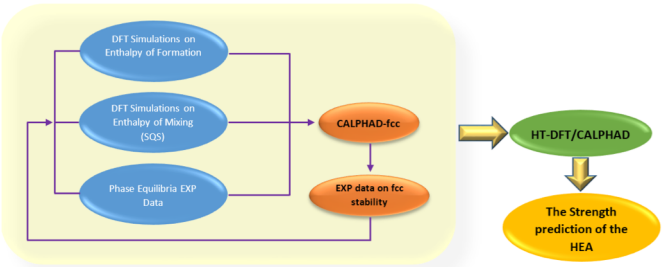
Project Objective & Scope

- Develop a predictive map on the strength of Fe-Ni-Cr-Co high entropy alloy single crystals, applying integrated HT-DFT/CALPHAD approach.

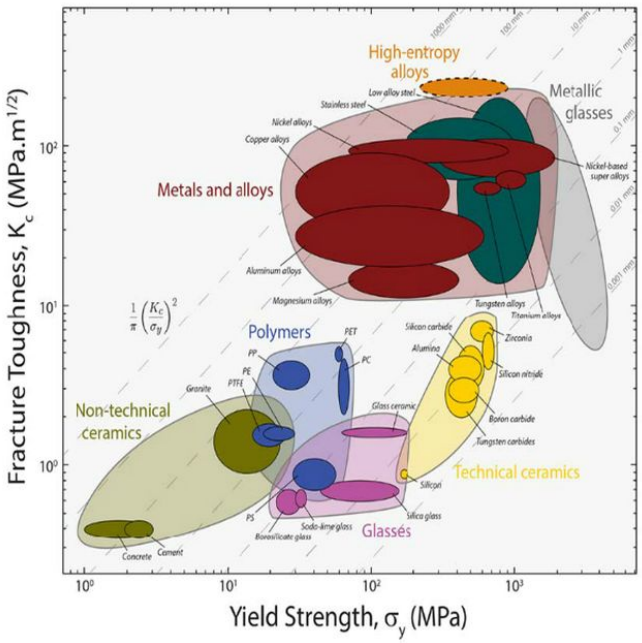
Anticipated Project Benefits/Approach

- Development of a model that is capable to predict the strength of different compositions of Fe-Ni-Cr-Co high entropy alloy single crystals can considerably enhance materials selection process for the design of high performance structural alloys in different systems like Fossil Energy (FE) power plants.



Introduction

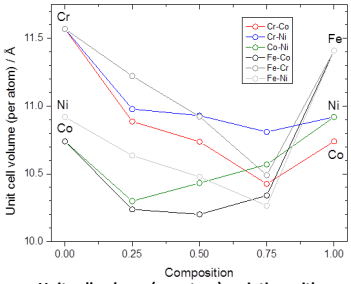
- High entropy alloys (HEAs) have been considered recently due to their interesting properties such as high strength, high hardness, high temperature softening resistance, etc. Fe-Ni-Cr-Co is one of the attractive HEAs due to its special properties. For example, contrary to the most traditional materials, Fe-Ni-Cr-Co shows simultaneous increase in both strength and ductility by decreasing temperature.
- In order to be able to apply Fe-Ni-Cr-Co system as a high performance structural material, different properties of this system at various conditions should be known. One of the most important properties of this material is strength. Therefore, a predictive map to show the strength of Fe-Ni-Cr-Co system with different compositions is required.



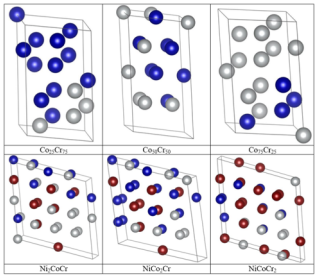
Ashby map showing fracture toughness vs. yield strength (Gludovatz et al., 2014)

Computational Details

- ✓ ***Special quasi-random structure (SQS) generation-*** Binary and ternary SQS structures for the random *fcc* alloys in Fe-Ni-Co-Cr system were generated using *gensqs* code in the Alloy-Theoretic Automated Toolkit (ATAT). Face-centered cubic unit cells contained 16 and 32 atoms for binary and ternary systems, respectively.
- ✓ ***DFT-*** Density functional theory (DFT) calculations were performed using Vienna ab initio simulation package (VASP). The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) exchange-correlation functional was used to describe exchange and correlation effects. Electron wave functions were expanded by plane wave with a cutoff energy of 500 eV. Monkhorst-Pack k-point meshes with density not less than 1000 pra (per-reciprocal-atom) were used to sample the Brillouin zones. Both cutoff energy and k-point mesh were tested to achieve a sufficiently high accuracy. Atomic relaxation was performed until the change in total energy was less than 0.01 meV, and all of the forces on each atom were smaller than 0.01 eV/Å. For elastic properties calculations cutoff energy and density of k-points mesh were increased to 700 eV and 7000 eV, respectively. Total energy of pure metals was calculated for their most stable crystal form at ambient conditions.



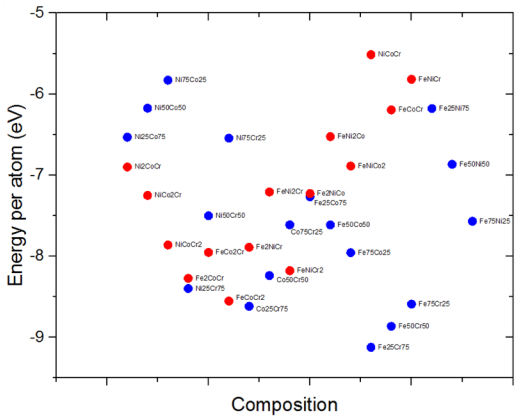
Unit cell volume (per atom) variation with composition in binary systems Fe-Ni-Co-Cr



Relaxed crystal structure of some binary and ternary alloys in Ni-Co and Ni-Co-Cr systems

Calculated lattice parameters and unit cell volumes of some binary and ternary alloys in Co-Cr and Ni-Co-Cr system

Alloy	a, Å	b, Å	c, Å	α, °	β, °	γ, °	V, Å^3	E, eV
$Co_{25}Cr_{75}$	4.28658	5.56248	7.50846	98.6822	95.5930	97.5124	174.20	-8.617072
$Co_{50}Cr_{50}$	4.29748	4.94724	8.20461	89.2650	99.8064	90.3449	171.80	-8.238287
$Co_{75}Cr_{25}$	4.25776	5.45924	7.36636	98.6792	95.5490	97.0561	166.82	-7.612148
Ni_2CoCr	8.57648	8.54993	4.93536	89.9540	89.8667	109.6309	340.87	-220.7639510
$NiCo_2Cr$	8.52125	8.51897	4.91520	90.0019	89.9556	109.4659	336.41	-232.0104550
$NiCoCr_2$	8.60913	8.63089	4.96688	90.1180	89.7492	109.6964	347.46	-251.5637870



Total energy (per atom) for binary and ternary alloys in Fe-Ni-Co-Cr system

Acknowledgment

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