AOI 3: High Throughput Computational Framework of Materials Properties for Extreme Environments

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Project Objectives and Benefits

This project aims to establish a framework capable of efficiently predicting the properties of structural materials for service in harsh environments. An integrated approach is adopted including high throughput first-principles calculations in combination with machine learning, high throughput calculations of phase diagrams (CALPHAD), and finite element method (FEM) simulations. Relevant to high temperature service in fossil power system, Ni-based superalloys Inconel 740 and Haynes 282 as well as the associated (Ni-Cr-Co)-Al-C-Fe-Mn-Mo-Nb-Si-Ti alloy system, will be investigated.

This framework enables high throughput computation of tensile properties of multicomponent alloys at elevated temperatures, resulting in significant reduction in computational time needed by the state-of-the-art methods. Once successfully completed, the project will deliver an open-source framework for high throughput computational design of multicomponent materials under extreme environments. This framework will enable more rapid design of materials and offer the capability for further development of additional tools due to its open-source nature.

Overview of Computational Approach

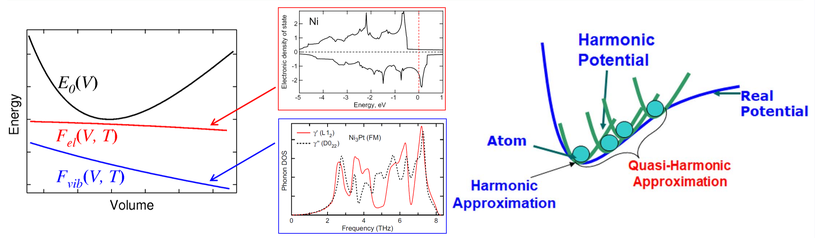
Atomate/WEKA → First-principles calculations → ESPEI: High throughput CALPHAD → Pycalphad: Computation engine → ABAQUS: FEM

- ✓ Predict thermodynamic and other properties using DFT and CALPHAD
- ✓ Use machine learning to reduce the number of first-principle calculations
- ✓ Apply FEM to simulate tensile strength
- ✓ Validate results and improve models

First-Principles Calculations

$$F(V,T) = E_0(V) + F_{vib}(V,T) + F_{el}(V,T)$$

- $E_0(V)$ Static energy at 0 K and volume V, i.e., EOS (by DFT directly, VASP)
- $F_{vib}(V,T)$ Vibrational contribution at V & T (Phonon, TFC, or Debye)
- $F_{el}(V,T)$ Thermal electronic contribution at V & T (by DFT directly, VASP)



Prediction of finite temperature properties of materials

High Throughput First-Principles Calculations

- Materials analysis and I/O (Pymatgen)
- Calculation error recovery (Custodian)
- Workflow package (FireWorks)

→ Materials calculate environment (*Atomate*)

- Allows large scale calculations in an efficient way
- Allows greater control and automation of VASP
- Allows for the introduction of machine learning

CALPHAD Modeling

The CALPHAD method is to model Gibbs energy of individual phases using both thermodynamic data of single phase and phase equilibrium data between phases. The CALPHAD approach has been extended to model such as elastic properties, molar volumes, stacking fault energy, and diffusion coefficients of multicomponent alloys via input from experiments and first-principles.

Derivatives of Gibbs energy → Thermochemical data: heat capacity, enthalpy, entropy, activity

$D_{ip}d\xi=0$ → Phase equilibrium data: phase stability, phase boundary

CALPHAD 1973

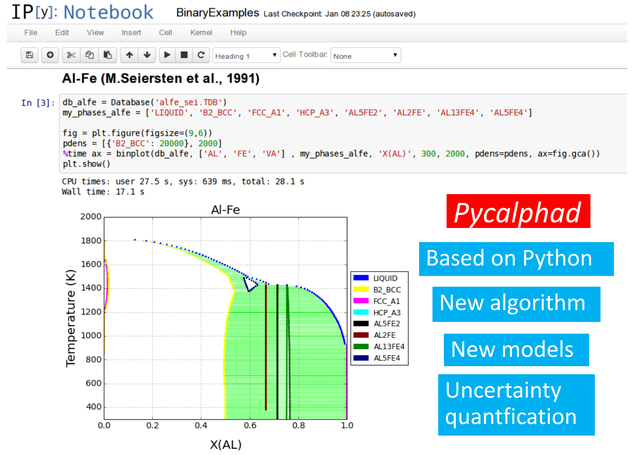
Gibbs Energy of Individual Phases $G^{\Phi}(T,P,N_i,\xi)$

Applications: Equilibrium, driving force, physical/chemical properties (1st, 2nd derivatives)

ESPEI *pycalphad*

Pure elements → Binary → Ternary → Multicomponent

High Throughput CALPHAD Modeling



ESPEI-2.0 Software Stack

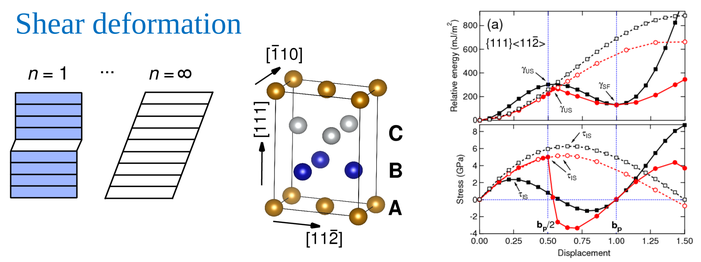
- ESPEI
- *pycalphad*
- NumPy
- SymPy

Pycalphad

- Based on Python
- New algorithm
- New models
- Uncertainty quantfication

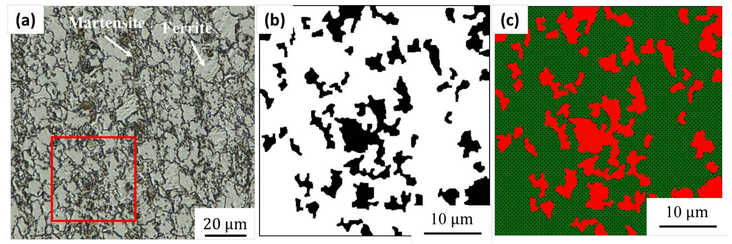
Prediction of properties

Shear deformation



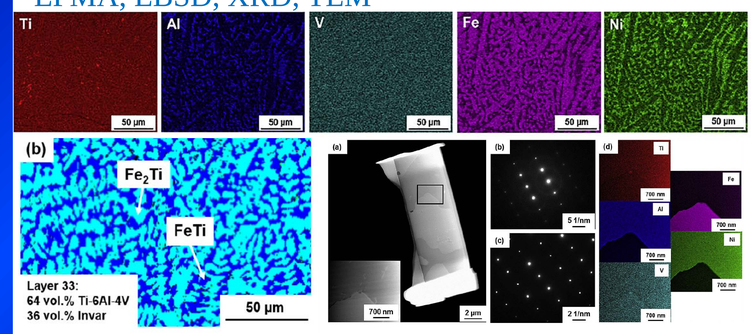
FEM simulations

Representative Volume Element (RVE): Crystal Plasticity Simulations



Experimental Characterization

EPMA, EBSD, XRD, TEM



Summary

A high throughput multiscale computational framework is used to simulate materials properties under extreme environments.

References

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[5] Liu & Wang, *Computational Thermodynamics of Materials* (2016).