High Throughput Computational Framework of Materials Properties for Extreme Environments

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Outline

- Overview of proposed goal and our approaches
- Results and discussion
  - A combined DFT/FEM approach to study stress-stain curve of single crystals
  - A combined DFT/FEM approach to study stress-stain curve of polycrystals
  - A combined DFT/ML approach to study key fundamental: Ideal shear strength of Ni-X (Ni$_{11}$X)
- Summary of achievements
Goal ⇒ To establish an open-source infrastructure for predictive modeling of materials properties at extreme environments, including:

• High throughput DFT-based first-principles calculations for properties of interest, including such as phonon, thermodynamic, elastic, ideal shear strength, and stacking fault properties;

• High throughput CALPHAD modeling of the above properties using our unique capability;

• New capabilities to predict the stress-strain behavior of single crystals and polycrystals; and

• Phase-based new models for tensile strength prediction using the common finite element method (FEM) analysis software.
Overview of high throughput computational framework for materials properties under extreme environments

- Predict proto data using DFT Tool Kit (DFTTK) and machine learning (SIPFENN)
- Apply FEM (ABAQUS) to predict strain-stress curve and tensile strength
- Use CALPHAD approach (ESPEI/PyCalphad) to predict processed data
- Validate results and improve models
**DFT/FEM \( \Rightarrow \)** stress-strain of single crystal

Dislocation interactions are the major strain hardening mechanism for fcc Ni

**At low strains**: long-range dislocation interactions dominate

**At high strains**: short-range dislocation interactions dominate

Dislocation interactions are realized in DFT-based calculations through the application of pre-strains

\[ \tau_{IS} = \sum_{\beta=1}^{l} h_{\alpha\beta} |\gamma^{\beta}| \]

**Slip system** (mesoscale)

**CPFEM simulations**

**FEA vs. Experiments** (macroscale)

Single crystal hardening model

The Peierls-Nabarro model

\[ \tau_P = \frac{Kb}{a} \exp\left(\frac{-2\pi Kb}{4\pi d \tau_{IS}}\right) \]

\( \tau_{IS} \) - Ideal shear strength from DFT-based calculations (is a function of pre-strains)

\( \tau_P \) - Flow resistance of a dislocation (the PN stress)

CPFEM (crystal plasticity finite element method) model

\[ \dot{\tau}_c^\alpha = \sum_{\beta=1}^{l} h_{\alpha\beta} |\dot{\gamma}_\beta| \]

\[ h_{\alpha\beta} = q_{\alpha\beta} \left( h_0 \operatorname{sech}^2 \left( \frac{h_0 \gamma}{\tau_s - \tau_0} \right) \right) \]

\( h_0, \tau_0, \) and \( \tau_s \) - CPFEM model parameters (determined from DFT-based predictions)

\( \gamma_\beta \) - Pre-strain applied in DFT-based calculations

\( \tau_c^\alpha \) - Flow resistance

At low strains (where edge dislocations dominate):

\[ \tau_c^\alpha = \tau_P^{edge} \]

At large strains (where both edge and screw dislocations are present):

\[ \tau_c^\alpha = (1 - w \gamma_\beta) \tau_P^{edge} + w \gamma_\beta \tau_P^{screw} \]

\( w \) - Weighting factor (=0.33, calibrated with macroscale experimental data)

Results ⇒ stress-strain of single crystal Ni

- CPFEM model parameters were calibrated from DFT-based predictions (except for the weighting parameter $w$)
- FEA using the calibrated CPFEM model agreed well with macroscale experiments

**Calibration of $w$**

Flat tensile specimen

$(2.5 \times 5.5 \times 0.25 \text{ mm}^3)$

- Experiment
- CPFEM

### Validation

- Experiment
- CPFEM

Stress strain curve

Strain hardening rate

**Round wire specimen**

Diameter = 2.24 mm
Length = 71.12 mm

Polycrystals: Bassani-Wu modification to single crystal model

\[ h_{\alpha\beta} = \{q - (q + 1)\delta_{\alpha\beta}\} \cdot \left\{ (h_0 - h_s) \text{sech}^2 \left[ \frac{(h_0 - h_s)\gamma}{\tau_s - \tau_0} \right] + h_s \right\} \cdot \left\{ 1 + \sum_{\beta \neq \alpha} f_{\alpha\beta} \tanh \left( \frac{\gamma^\beta}{\gamma_0} \right) \right\} \]

*Extra parameters from Bassani-Wu model in red*

**Single slip system behavior:**

**Polycrystal behavior:**

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137 grain polycrystal model

| 08: \( \tau_0 = 13, h_0 = 280, \tau_s = 30, h_s = 0.1, \gamma_0 = 0.25, f_0 = 1, q = 1 \) |
| 25: \( \tau_0 = 68, h_0 = 350, \tau_s = 80, h_s = 0.1, \gamma_0 = 0.25, f_0 = 1, q = 1 \) |

**Experimental data:**
- 2um
- 130um
Polycrystals: Automated optimization

Bayesian optimization is a machine learning based approach used for functions that are expensive to evaluate. It does not require gradients.

General example of Scikit-optimize:
https://scikit-optimize.github.io

Used to find optimal Bassani-Wu parameters that match experimental data for polycrystal nickel of different grain sizes
Alloys: Ideal shear strength of Ni-X (Ni\textsubscript{11}X)

- Extend pure Ni calculations by DFT-based alias shear deformation to binary Ni-X (Ni\textsubscript{11}X) substitutional solid solution
- Ni host with 26 alloying elements X
- To explain differences in ideal shear strength, look at alloying element descriptors & their associations

Example: Ni\textsubscript{11}V
Alloys: Sequential wrapper method, correlations

Instead of the common belief of shear modulus, we found the dominant effects of atomic volume and electronegativity on ideal shear strength.

Using a simple ML model, e.g. linear SVM:

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Forward variant: add features whose addition results in the lowest RMSE.

Colored according to frequency in top 10.
Summary

Multiscale approach from electron, atoms, to phase, and applications

- **High-throughput calculations for fast data-gain**
  - DFT-based first-principles calculations of thermodynamic/mechanical properties
  - CALPHAD modeling to develop the databases of interest
  - Python-based open source codes: SIPFENN, DFTTK, ESPEI, and PyCalphad

- **A combined DFT/FEM approach to study stress-stain curve and tensile strength for both single crystals and polycrystals**
  - Phase-based Crystal plasticity finite element method (CPFEM) for single crystals
  - Phase-based CPFEM for polycrystals (Bassani-Wu modification)
  - Key fundamental ⇒ Ideal shear strength of Ni and Ni$_{11}$X by DFT calculations and machine learning understanding