High Throughput Computational Framework of Materials Properties for Extreme Environments

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Outline

• Predictive crystal plasticity modeling of Ni single crystal based on first-principles calculations

• Density functional theory informed dislocation density hardening within crystal plasticity: Application to Ni polycrystals

• First-principles calculations of ideal shear strength for Ni-X-Z dilute multicomponent alloys
Overview of high throughput computational framework for materials properties under extreme environments

- Predict **proto data** using DFT Tool Kit ([www.DFTTK.org](http://www.DFTTK.org)) and machine learning models ([https://phaseslab.com/sipfenn/](https://phaseslab.com/sipfenn/))
- Apply FEM (ABAQUS) and dislocation density based FFT methods to predict tensile strain-stress curve
- Use CALPHAD approach (PyCalphad.org and ESPEI.org) to model **processed data**
- Validate results and improve models
Mechanical Behavior from First Principles

Physically-meaningful crystal plasticity parameters \(\rightarrow\) predictive framework for deformation

Shimanek et al. *JOM* 74 (2022) 1423-1434
- Elastic constants
- Ideal shear stress:
  - Alias shear – one layer involved
  - One lattice parameter fixed, all else relaxed
  - Needs a conversion to dislocation-mediated critical resolved shear stress

Joós-Duesbery Peierls-Nabarro model:

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

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

\( K \): anisotropic elastic factor, which depends on dislocation character

a, d: lattice periodicity length respectively within slip plane, between slip places

Describing Hardening at Finite Strain

Need to account for short range effects on dislocation motion – increased screw dislocation density within junctions with increase of strain

- Flow stress from $K^{\text{edge}} \rightarrow \tau_P^{\text{edge}}$ (low)
- Flow stress from $K^{\text{screw}} \rightarrow \tau_P^{\text{screw}}$ (high)

**Low strains** (edge dislocation behavior):
\[ \tau_c^{\alpha} = \tau_P^{\text{edge}} \]

**Large strains** (edge, screw, junction behavior):
\[ \tau_c^{\alpha} = (1 - w\gamma^\beta)\tau_P^{\text{edge}} + w\gamma^\beta\tau_P^{\text{screw}} \]
w - Weighting factor (0.33, calibrated with macroscale experimental data from Yao et al.)

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Experimental Comparison: Ni

- With accurate $\tau_0$ & $h_0$, can calibrate $\tau_s$
  - Based on Yao data (as is $w$) at one orientation
- Use these parameters to predict large strain response of new orientations:

![Graphs showing experimental and predicted stress-strain curves](image)

- $\tau_{c,es}$

- CPFEM • Experiment

  Reasonable agreement at large strains


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Extension to Alloys: Binary Ni-X (Ni_{11}X)

- Alias shear deformation to Ni-X (Ni_{11}X) solution
- 26 alloying elements
- Use alloying element descriptors to examine the variations of ideal shear strength

Example: Ni_{11}V

\[ \tau_{\text{ideal}} \]

Shear Stress, GPa

Displacement, Angstroms

arXiv: 2108.06412
## Ni$_{11}$X Correlational Study

- 26 Ni-based binary alloys, 45 atomic features
- Shown are five measures of association between pure atomic physical features and calculated ideal shear strength
- Several features in common:
  - Volume
  - Debye Temperature
  - Covalent radius
  - Electron density
  - Electronegativity
- Unexpected is the low importance of elastic constants

<table>
<thead>
<tr>
<th>Index</th>
<th>Regression Relief Algorithm</th>
<th>Coefficient of Determination</th>
<th>Maximal Information Coefficient</th>
<th>Backward Wrapper: SVM</th>
<th>Forward Wrapper: SVM</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Volume</td>
<td>Volume</td>
<td>Volume</td>
<td>Electronic conductivity</td>
<td>Volume</td>
</tr>
<tr>
<td>2</td>
<td>Electron Density</td>
<td>Electronegativity</td>
<td>Electronegativity</td>
<td>Volume</td>
<td>Debye Temperature</td>
</tr>
<tr>
<td>3</td>
<td>Mendeleev Number</td>
<td>Electron Density</td>
<td>Debye Temperature</td>
<td>No. F Valence Filled</td>
<td>G</td>
</tr>
<tr>
<td>4</td>
<td>Covalent Radius</td>
<td>Covalent Radius</td>
<td>E</td>
<td>Debye Temperature</td>
<td>Electronic Conductivity</td>
</tr>
<tr>
<td>5</td>
<td>Standard Entropy</td>
<td>Debye Temperature</td>
<td>G</td>
<td>Heat Capacity</td>
<td>No. F Valence Unfilled</td>
</tr>
<tr>
<td>6</td>
<td>Electronegativity</td>
<td>Pauling Electronegativity</td>
<td>Mendeleev Number</td>
<td>Electron Density</td>
<td>E</td>
</tr>
<tr>
<td>7</td>
<td>Pseudopotential Radius: s-shell</td>
<td>Mendeleev Number</td>
<td>Covalent Radius</td>
<td>Covalent Radius</td>
<td>Electronegativity</td>
</tr>
<tr>
<td>8</td>
<td>Pseudopotential Radius: p-shell</td>
<td>G</td>
<td>Electron Density</td>
<td>No. Valence Filled</td>
<td>Heat of Sublimation</td>
</tr>
<tr>
<td>9</td>
<td>Electron Range</td>
<td>E</td>
<td>No. D Valence Filled</td>
<td>No. P Valence Filled</td>
<td>B</td>
</tr>
<tr>
<td>10</td>
<td>Debye Temperature</td>
<td>No. Valence Unfilled</td>
<td>Group</td>
<td>Mass</td>
<td>Boiling Temperature</td>
</tr>
</tbody>
</table>

Index: 1-10

Coefficients: Regression, Relief, Coefficient of Determination, Maximal Information Coefficient, Backward Wrapper: SVM, Forward Wrapper: SVM

arXiv: 2108.06412
## Ternary Ni-X-Z (Ni$_{34}$XZ) Ideal Shear Stress

### Strengthening elements
- Co: 5.24
- Mn: 5.17
- Fe: 5.15
- Cr: 5.15
- Al: 4.73
- Ti: 4.55
- Mo: 4.45
- Si: 4.31
- Nb: 4.16

### Softening elements
- (Pure Ni$_{36}$: 5.10 GPa)
- Co: 5.20
- Mn: 5.07
- Fe: 5.05
- Cr: 4.86
- Al: 4.63
- Ti: 4.51
- Mo: 4.41
- Si: 4.31
- Nb: 4.17

### Deviation from fit above indicates nonlinear effects not captured in equation below:

$$\tau_{i_d}^{linear}(Ni_{34}XZ) = 0.5 \tau_{i_d}(Ni_{34}X_2) + 0.5 \tau_{i_d}(Ni_{34}Z_2)$$
### Ni$_{34}$XZ Correlational Study

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<tr>
<th>Index</th>
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</tr>
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<tr>
<td>1</td>
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<td>Volume</td>
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<td>Volume</td>
</tr>
<tr>
<td>2</td>
<td>B$_{DFT}$</td>
<td>Van der Waals atomic radius</td>
<td>G/B$_{DFT}$</td>
<td>B$_{DFT}$</td>
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<tr>
<td>3</td>
<td>G/B$_{DFT}$</td>
<td>Boiling Temperature</td>
<td>Cohesive energy</td>
<td>Cohesive energy</td>
</tr>
<tr>
<td>4</td>
<td>Heat of Fusion</td>
<td>The third ionization potential</td>
<td>B$_{DFT}$</td>
<td>G/B$_{DFT}$</td>
</tr>
<tr>
<td>5</td>
<td>Cohesive energy</td>
<td>Elastic constant C$_{12, DFT}$</td>
<td>Vaporization heat</td>
<td>Heat of Sublimation</td>
</tr>
<tr>
<td>6</td>
<td>Mass</td>
<td>Heat of Sublimation</td>
<td>Elastic constant C$_{44, DFT}$</td>
<td>Poisson ratio</td>
</tr>
<tr>
<td>7</td>
<td>Heat of Sublimation</td>
<td>Cohesive energy</td>
<td>Heat of Sublimation</td>
<td>Mass</td>
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<td>8</td>
<td>Number of valence electron</td>
<td>The first ionization potential</td>
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<td>Heat of Fusion</td>
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<tr>
<td>9</td>
<td>Van der Waals atomic radius</td>
<td>Elastic constant C$_{13, DFT}$</td>
<td>Number of valence electron</td>
<td>Square root of B/G</td>
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<td>Square root of B/G</td>
<td>Vaporization heat</td>
</tr>
</tbody>
</table>

- 45 Ni-based ternary alloys, 80 physical features
- Several features in common:
  - Volume (agree with Ni-X study)
  - Ratio between shear modulus and bulk modulus
  - Cohesive energy
  - Bulk modulus
  - Vaporization heat

![Graph](image)
Extension of PAN-CPFEM to Polycrystals

1. Simplified polycrystal microstructures:

2. Automated parameter optimization:

3. Grain size dependence shows power law behavior for all hardening parameters.

Exponent varies with material, may correlate with material properties such as stacking fault energy (shown to right).

4. Slow performance and unclear physical interpretations motivates move from CPFEM using PAN to FFT using dislocation density hardening law.
Crystal plasticity fast Fourier transform (CPFFT)

CPFFT explicitly models the microstructure, individual grains, slip systems and their interactions to capture the micromechanical anisotropy of polycrystals.

High-performance CPFFT

~400x speed up on 10 Tesla V100 GPUs
Orders of magnitude faster than CPFEM
Original dislocation density (DD) hardening

\[ \tau_c^s = \tau_0^s + \tau_{for}^s + \tau_{deb}^s \]

\[ 0.9\mu b \sqrt{\rho_{for}^s + 1.05 \sum_{s=1}^S \rho_{for}^s} \]

\[ 0.086 \mu b \rho_{deb} \log \left( \frac{1}{\sqrt{\rho_{deb}}} \right) \]

\[ \frac{\partial \rho_{for}^s}{\partial \gamma} = k_1 \sqrt{\rho_{for}^s} - k_2 \rho_{for}^s \]

\[ \frac{\partial \rho_{deb}}{\partial \gamma} = q \sum_s b \sqrt{\rho_{deb} k_2 \rho_{for}^s} \]

\[ k_2 = 0.9 k_1 b \frac{1}{\gamma} \left( 1 - \frac{K_B T}{D \beta^3} \ln \left( \frac{\varepsilon}{\varepsilon_0} \right) \right) \]

DFT-informed DD hardening

\[ g = \frac{\Delta \Gamma_{SFE}}{\mu b_{\langle \{11\} \rangle}} = \frac{\Gamma_{USFE} - \Gamma_{ISFE}}{\mu b_{\langle \{11\} \rangle}} \]

\[ q = \frac{H_{f, Va}}{16 \mu b^{3}_{\langle \{11\} \rangle} g} \]

Calibration

\[ \tau_0^s, k_1, D, g, q \]

True stress [MPa] vs. True strain

Normalized activation energy

Rate of dislocation debris

\[ g, D, q \]

\[ k_1 \]

\[ \tau_0^s \]

\[ \frac{2\hat{b}_x^s + \hat{b}_y^s + \hat{b}_z^s}{(4d_{\text{grain}})} \]

\[ b \] Burgers vector

\[ \mu \] Shear modulus

Normalized activation energy

Calibration

DFT

\[ \tau_0^s, k_1, D \]

\[ g, q \]

\[ \frac{\Gamma_{USFE}}{\mu b_{\langle \{11\} \rangle}} \]

\[ \frac{\Gamma_{ISFE}}{\mu b_{\langle \{11\} \rangle}} \]

\[ H_{f, Va} \] vacancy formation energy

\[ \Gamma_{USFE} \] unstable stacking fault energy

\[ \Gamma_{ISFE} \] intrinsic stacking fault energy

\[ \hat{b} \] slip system

\[ \rho_{for} \] forest dislocations [mobile]

\[ \rho_{deb} \] debris dislocations [sessile]
DFT-Informed CPFFT

Density functional theory

Dislocation density hardening

FCC slip systems

Eng. stress [MPa]

Grain size [um]:
- 0.96
- 2.00
- 36.0

Polycrystalline deformation

Single crystal of many voxels
Simulation of flow response in polycrystalline Ni as a function of grain size
Correlating calibrated DD parameters with grain size

(i) $\gamma_p$ [MPa] vs. Grain size [$\mu$m]

(ii) $k_f$ [m$^{-1}$] vs. Grain size [$\mu$m]

(iii) $D$ [MPa] vs. Grain size [$\mu$m]

(a) $R^2=0.91$, $RMSE=0.46$

(b) $R^2=0.40$, $RMSE=0.12$

(c) $R^2=0.91$, $RMSE=0.13$
Identification of micromechanical hotspots

- Full-field CPFFT model offers **quantification of micromechanical fields**
- Provide insights into micromechanical **micro-crack incubation zones**
- Assist with **microstructure sensitive design** for performance optimization
Correlation of microstructural descriptors with full-field hotspots

- Descriptors
  - m´
  - Schmid factor
  - Orientation
  - Misorientation
  - Grain morphology
  - Grain boundary morphology

- Fields
  - Equivalent stress
  - Stress triaxiality
  - Equivalent plastic strain
  - Dislocation density
Microstructural descriptors

(a) 

(b) 

(c) 

(d) 

(i) GB surface  
(ii) triple junction  
(iii) quadruple point  

(e) 

(f) 

(g)
Local misorientation and $m'$ at grain boundary (GB)

$m'$ indicates the slip transmissibility at GBs

$0 \leq m' = \cos \kappa \cos \psi \leq 1$

$m' = 0 = \text{Impenetrable GB for slip transfer}$

$m' = 1 = \text{Slip is fully transmissible}$

$$\theta = \cos^{-1} \left( \frac{\sum_i \Delta g_{ii}^{AB} - 1}{2} \right)$$

$$\Delta g_{ij}^{AB} = (g_{ij}^A)^{-1} g_{ij}^B$$
Grain Morphology

(a) equiaxed
(b) elongated
(c) equiaxed grains with contrast in size.
(d) mix of equiaxed and elongated
(e) mix of equiaxed and elongated with contrast in size and shape.
Estimating microstructural feature importance on stress hotspots using machine learning: Random forest and SHapley Additive explanation (SHAP)

(a) Hotspots in Ni microstructure after uniaxial deformation to 2.5% strain

(b) Feature importance

SHAP value

M misorientation
M_prime
r_QP
Gr_size
S_nid
r_101
r_111
r_GB
Gr_shape
r_001
Summary

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

- High-throughput calculations and modeling for efficient data generation
  - DFT-based first-principles calculations of thermodynamic/mechanical properties
  - Machine learning models to predict and analyze properties
  - CALPHAD modeling to develop the databases
  - Python-based open-source codes: SIPFENN, DFTTK, PyCalphad and ESPEI

- A combined DFT/CP approach to study tensile stress-stain behaviors
  - Crystal plasticity finite element method (CPFEM) for single crystals with a phenomenological hardening law (PAN)
  - Ideal shear strength of alloys, Ni$_{11}$X and Ni$_{34}$XZ, by DFT calculations and machine learning models
  - DFT-informed hardening model based on dislocation densities, efficiently implemented through FFT for larger scale polycrystal calculations
K-fold cross-validation (KCV)

Cross-validation is a statistical technique used to evaluate the suitability of a model type. Errors for models tested on each fold are averaged and compared across models.

(a) Graphs showing the relationship between grain size and various parameters with $R^2$ values and RMSE for each fold. 
(b) Bar graphs showing RMSE values for each fold.