High Throughput Computational Framework of Materials Properties for Extreme Environments

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Outline

- Overview of proposed goal and technical approaches
- Results and discussion
  - A comprehensive DFT study of key fundamental properties: Ideal shear strength of pure elements, binary Ni-X (Ni_{11}X), and ternary Ni-X-Y (Ni_{34}XY) systems
  - A combined DFT/FEM approach to study constitutive behavior of single crystals and polycrystals
  - Machine learning models of materials properties: Illustrated with stacking fault energy
  - Development of hardness model
- 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 phonon, thermodynamic, elastic, ideal shear strength, and stable/unstable stacking fault properties related to Ni-based superalloys (e.g., Inconel 740);
- Exploration of machine learning models to predict the above properties;
- High throughput CALPHAD modeling of properties using our unique capability;
- New capabilities to predict the tensile stress-strain behavior of single crystals and polycrystals using finite element method (FEM) analysis; and
- Modeling of hardness with attributes from plastic deformations.
Overview of high throughput computational framework for materials properties under extreme environments

- Apply FEM (ABAQUS) to predict tensile strain-stress curve
- Use CALPHAD approach ([PyCalphad.org](https://PyCalphad.org) and [ESPEI.org](https://ESPEI.org)) to model processed data
- Validate results and improve models
DFT calculations of *generalized stacking fault energy*

**Alias shear deformation of fcc metals along \(<11\bar{2}>\) \{111\)**

- \(\gamma_{SF}\): Stacking fault energy
- \(\gamma_{US}\): Unstable stacking fault energy
- \(\tau_{IS}\): Ideal shear strength

### Ideal shear strength of pure elements (GPa)

#### Green (low value) – Yellow (middle) – Red (high)

| Elements | Type | E | Na | K | Al | Rb | Cs | Ce | Pr | Nd | Sm | Eu | Gd | Tb | Dy | Ho | Er | Tm | Yb | Lu |
|----------|------|---|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| Li 3     | 14.00| 0.20|    |    | 2.66|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| Be 4     | 5.22 | 0.15|    |    | 8.07|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 0.40     | 15.09| 0.40|    |    | 4.01|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| Na 11    | 0.61 | 0.44|    |    | 2.09|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| Mg 12    | 1.50 | 0.09|    |    | 2.09|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 0.19     | 1.50 | 0.19|    |    | 2.09|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
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| 0.19     | 1.50 | 0.19|    |    | 2.09|    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |

(Diamond: C, Si, Ge)
Ideal shear strength: Binary Ni-X (Ni\textsubscript{11}X)

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

Example: Ni\textsubscript{11}V

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

<table>
<thead>
<tr>
<th>21 Sc</th>
<th>22 Ti</th>
<th>23 V</th>
<th>24 Cr</th>
<th>25 Mn</th>
<th>26 Fe</th>
<th>27 Co</th>
<th>28 Ni</th>
<th>29 Cu</th>
<th>30 Zn</th>
<th>13 Al</th>
<th>14 Si</th>
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</thead>
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<tr>
<td>39 Y</td>
<td>40 Zr</td>
<td>41 Nb</td>
<td>42 Mo</td>
<td>43 Tc</td>
<td>44 Ru</td>
<td>45 Rh</td>
<td>46 Pd</td>
<td>47 Ag</td>
<td>48 Cd</td>
<td>49 In</td>
<td>50 Sn</td>
</tr>
<tr>
<td>71 Lu</td>
<td>72 Hf</td>
<td>73 Ta</td>
<td>74 W</td>
<td>75 Re</td>
<td>76 Os</td>
<td>77 Ir</td>
<td>78 Pt</td>
<td>79 Au</td>
<td>80 Hg</td>
<td>81 Tl</td>
<td>82 Pb</td>
</tr>
</tbody>
</table>

Shear Stress, GPa vs. Displacement, Angstroms
Ideal shear strength: Ternary Ni-Z-X (Ni$_{34}$ZX)

• Supercell: 36-atom with 3 {111} layers
• Total Ni$_{34}$FeX configurations $\rightarrow$ 39
• 0.05 (Si) ~ 0.25 (Mn) GPa spread due to positions of Z and X in the supercell
Multiscale predictive simulation: Single crystal

DFT-based predictions

Slip system hardening

Crystal plasticity

Key contributions: Flow resistance

• Predicted by elastic properties and ideal shear strength based on the Peierls-Nabarro model

• At low strains: Edge dislocation

\[ \tau_c^\alpha = \tau_{\text{P}} \]

• At large strains: Junctions with screw components

\[ \tau_c^\alpha = (1 - w\gamma^\beta)\tau_{\text{P}}^{\text{edge}} + w\gamma^\beta \tau_{\text{P}}^{\text{screw}} \]
Stress-strain behavior of Ni: Single crystal

- \( h_{\alpha\beta} = q_{\alpha\beta} \left[ h_0 \, \text{sech}^2 \left( \frac{h_0 \gamma}{\tau_s - \tau_0} \right) \right] \)
  - \( \tau_0 \) & \( h_0 \) from DFT predictions
  - \( w \) and \( \tau_s \) calibrated to Yao data

- Predict large strain response of various orientations (Haasen data)

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Ni-X stress-strain behavior

First-principles results considering pre-strain.
Resolved shear stress calculated using:
\[ \tau^\alpha_c = (1 - w\gamma^\beta)\tau^{edge}_P + w\gamma^\beta\tau^{screw}_P \]
Polycrystal hardening moduli

• Pierce-Asaro-Needleman
  • Function of $\gamma = \Sigma\gamma^\beta$
  • Three parameters: $\tau_0$, $h_0$, $\tau_s$
  • Limited hardening capacity

• Bassani-Wu
  • Function of $\gamma^\beta$
  • Two additional parameters
  • Higher hardening capacity

• Modified PAN
  • Function of $\gamma^\beta$
  • Three parameters
  • Higher hardening capacity
Polycrystal models

• Simplified polycrystal models
  • Accurate to larger microstructural models
  • Much more efficient

• Automated parameter search
  • Existing open-source optimization library, scikit-optimize (scikit-optimize.github.io)
  • No gradient information necessary (Bayesian optimization via Gaussian processes)
  • Independent of hardening model details

• Hardening model conclusions
  • PAN increased hardening capacity when using $\gamma^B$
  • Grain size dependence from literature on Ni, Cu
Correlation analysis of materials properties by **machine learning**: Stacking fault energy in dilute fcc-based alloys

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**Figure (a)**: Graph showing the average MAE (mJ/m$^2$) versus the number of descriptors employed.

**Figure (b)**: Scatter plot comparing the change in stacking fault energy ($\Delta \gamma_{SFE}$) of Pt$_{23}X$ by DFT (mJ/m$^2$) against the change in stacking fault energy ($\Delta \gamma_{SFE}$) of FCC alloys by ML. The linear fit is shown with $R^2 = 0.81$.

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Temperature-dependent hardness model

\[ H_v = 0.1615 \frac{b}{G} \left( 1 + 5200 \frac{b}{(1 - v)^2 w(T)} \right)^2 \left( \frac{T_{PN}}{G(T)} \right)^4 \left( \frac{1}{1.4} \right)^2 \exp \left( -2.2k \left( 1 - v \right) \frac{b}{w(T)} \right) \tan^{3/2} \alpha \cos \alpha \]

- Thermally activated dislocation motion: Correlated to diffusion
- For most FCC metals
  - At high-T, dislocation climb
  - At low-T, dislocation glide
Hardness model for twin boundary

• For FCC metals:
  \[ b \left( \frac{1}{2} [110] \right) \rightarrow b_1 \left( \frac{1}{2} [110]_T \right) + b_2 \left( \frac{1}{6} [11\bar{2}] \right) \]

• Dislocation through twin boundary \( \Rightarrow \) Shockley partial dislocations \( \left( \frac{1}{6} [11\bar{2}] \right) \) activated near twin boundaries \( \Rightarrow \) screw characteristics

a) FCC Copper
b) FCC Silver
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 of interest
  - CALPHAD modeling to develop the databases
  - Python-based open-source codes: SIPFENN, DFTTK, ESPEI, and PyCalphad

- A combined DFT/FEM approach to study tensile stress-stain behaviors for both single crystals and polycrystals
  - Crystal plasticity finite element method (CPFEM) for single crystals
  - CPFEM for polycrystals (Modified PAN model)
  - Key fundamental ➔ Ideal shear strength of pure elements, Ni_{11}X, Ni_{34}ZX by DFT calculations and machine learning understanding
  - Hardness model ➔ Considering both elastic and plastic deformations temperature, and cross-slip mechanism of dislocation