High Throughput Computational Framework of Materials Properties for Extreme Environments

PIs: Zi-Kui Liu, Allison Beese, and Shun-Li Shang
Researchers: Shipin Qin, John Shimanek, and Yi Wang

Department of Materials Science and Engineering
The Pennsylvania State University, PA 16802

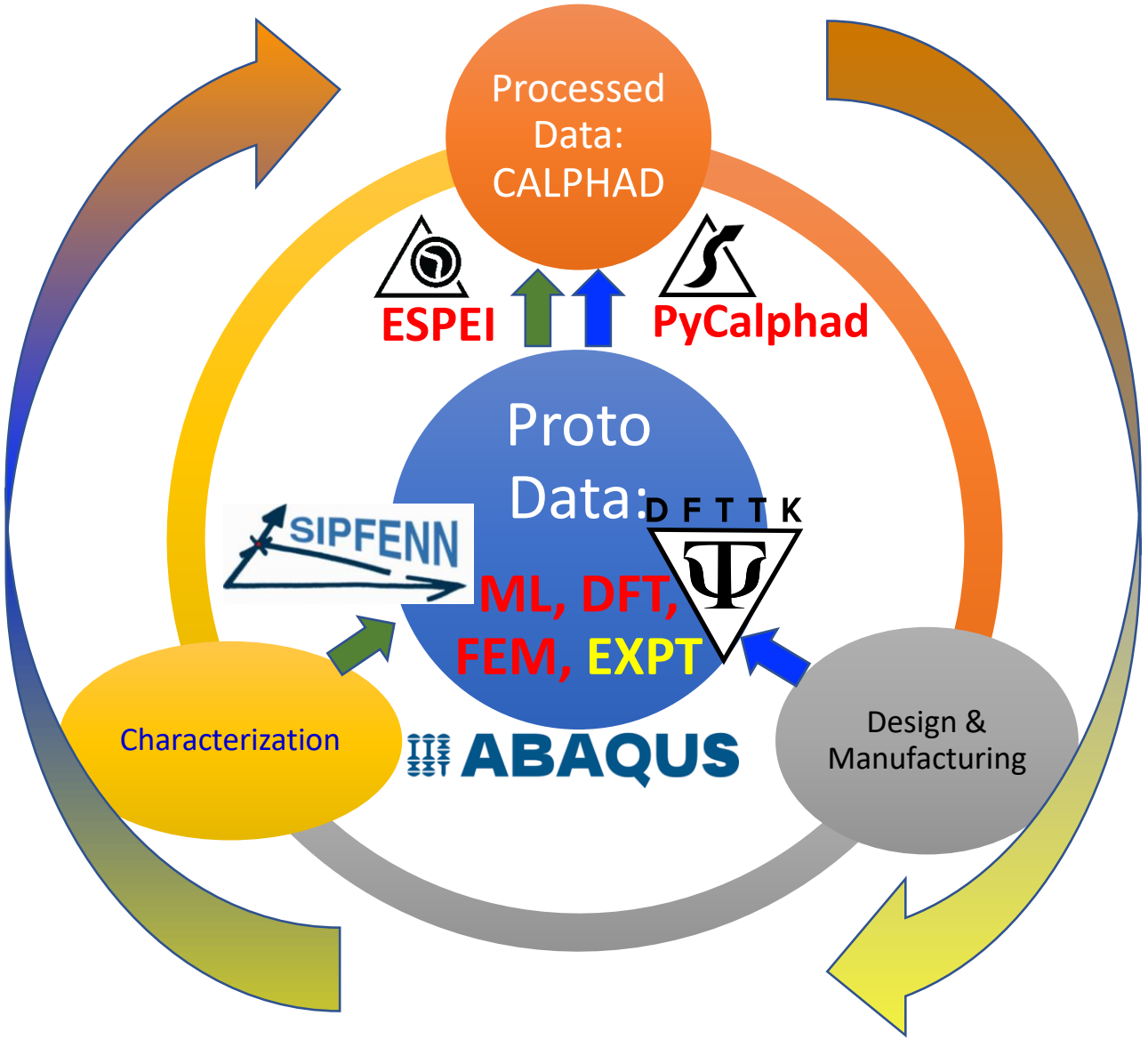
Outline

- 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 ploycrystals; 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

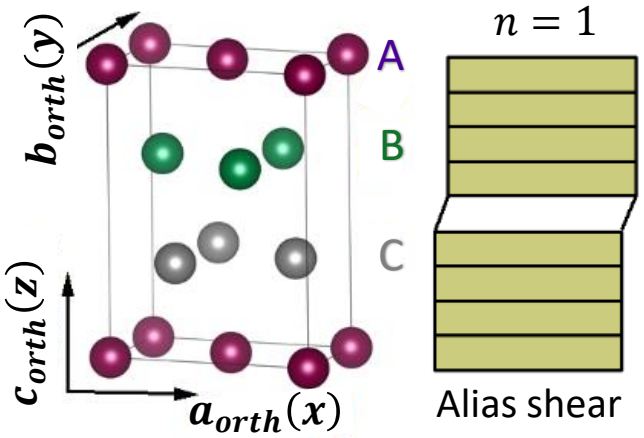


- ✓ Predict proto data using DFT Tool Kit (DFTTK) and machine learning (SIPFENN)
- ✓ Apply FEM (ABAQUS) to predict strain-stress curve and tensile strength
- ✓ Use CALPHAD approach (ESPEI/PyCalphad) to predict processed data
- ✓ Validate results and improve models

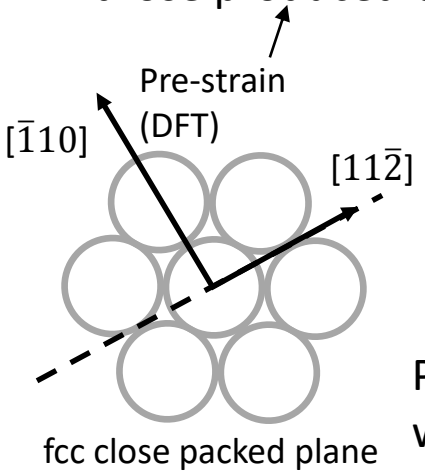
DFT/FEM ⇒ stress-strain of single crystal

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



Creates a strain field to mimic those produced by dislocations

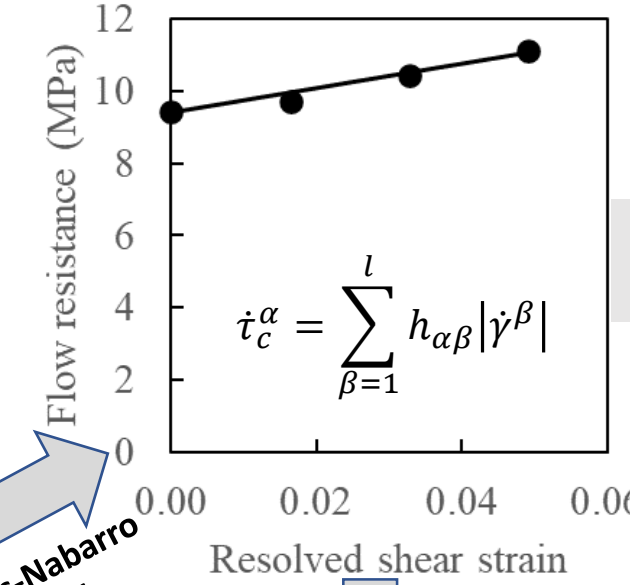


Alias shear to predict ideal shear strength τ_{IS}

Probe the τ_{IS} value with the influence of strain fields

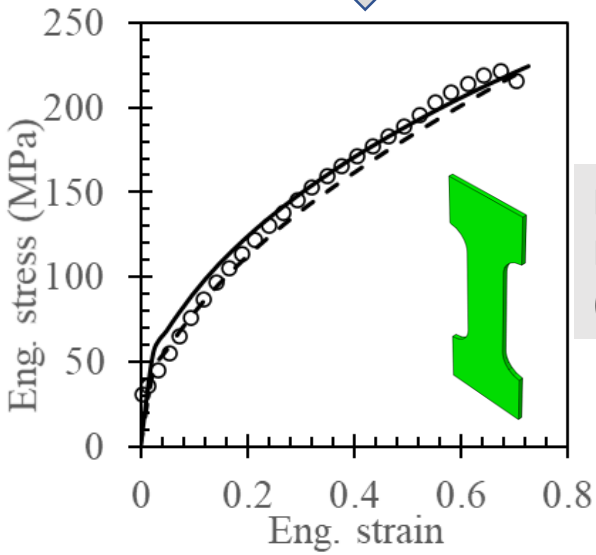
DFT-based predictions (atomic scale)

Peierls-Nabarro model



Slip system (mesoscale)

CPFEM simulations



FEA vs. Experiments (macroscale)

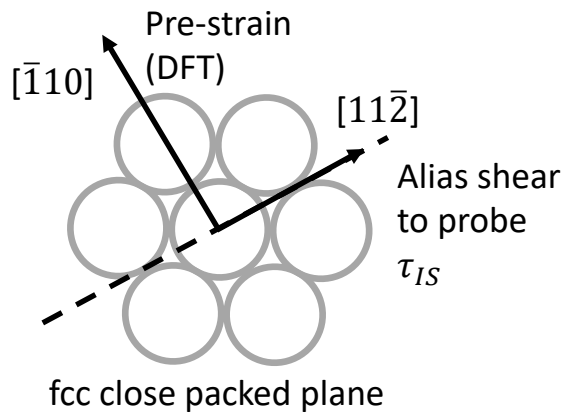
L. P. Kubin, et al. *J. Comput. Mater. Des.*, 1998.
S. I. Rao, et al., *Acta Mater.*, 2019

Single crystal hardening model

The Peierls-Nabarro model

$$\tau_{\mathrm{P}} = \frac{Kb}{a}\exp\left(\frac{-2\pi Kb}{4\pi d\tau_{\mathrm{IS}}}\right)$$

τ_{IS} - Ideal shear strength from DFT-based calculations (is a function of pre-strains)
τ_{P} - Flow resistance of a dislocation (the PN stress)



CPFEM (crystal plasticity finite element method) model

$$\dot{\tau}_c^{\alpha} = \sum_{\beta=1}^{l} h_{\alpha\beta}\left|\dot{\gamma}^{\beta}\right|$$

$$h_{\alpha\beta} = q_{\alpha\beta}\left[h_0\,\mathrm{sech}^2\left|\frac{h_0\gamma}{\tau_s - \tau_0}\right|\right]$$

h_0, τ_0, and τ_s - CPFEM model parameters (determined from DFT-based predictions)
γ^{β} - Pre-strain applied in DFT-based calculations
τ_c^{α} - Flow resistance

At **low strains** (where edge dislocations dominate):

$$\tau_c^{\alpha} = \tau_{\mathrm{P}}^{edge}$$

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

$$\tau_c^{\alpha} = \left(1 - w\gamma^{\beta}\right)\tau_{\mathrm{P}}^{edge} + w\gamma^{\beta}\tau_{\mathrm{P}}^{screw}$$

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

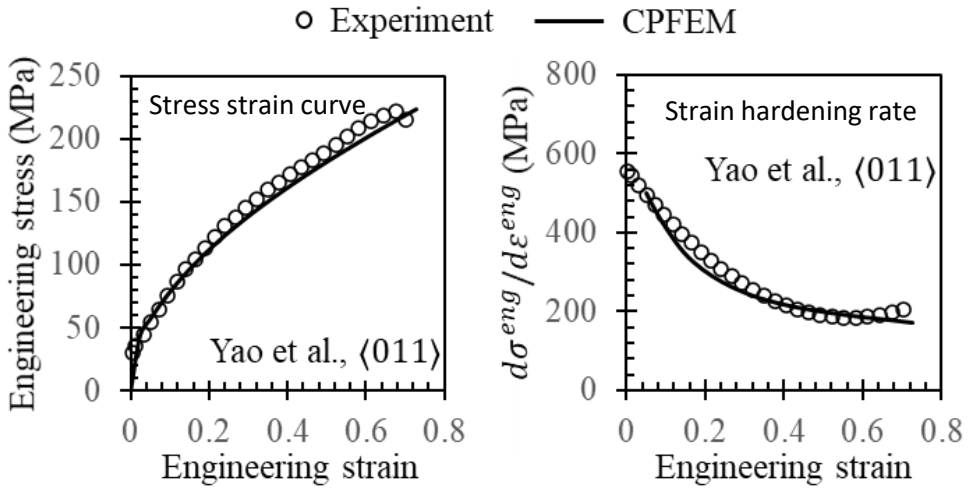
B. Joós et al., *Phys. Rev. Lett.*, 1997.
Y. Huang, *Harvard Univ.*, 1991.
D. Peirceet al., *Acta Metall.*, 1982.
S. Qin et al., *arXiv preprint arXiv, 2020.*

Results ⇒ stress-strain of single crystal Ni

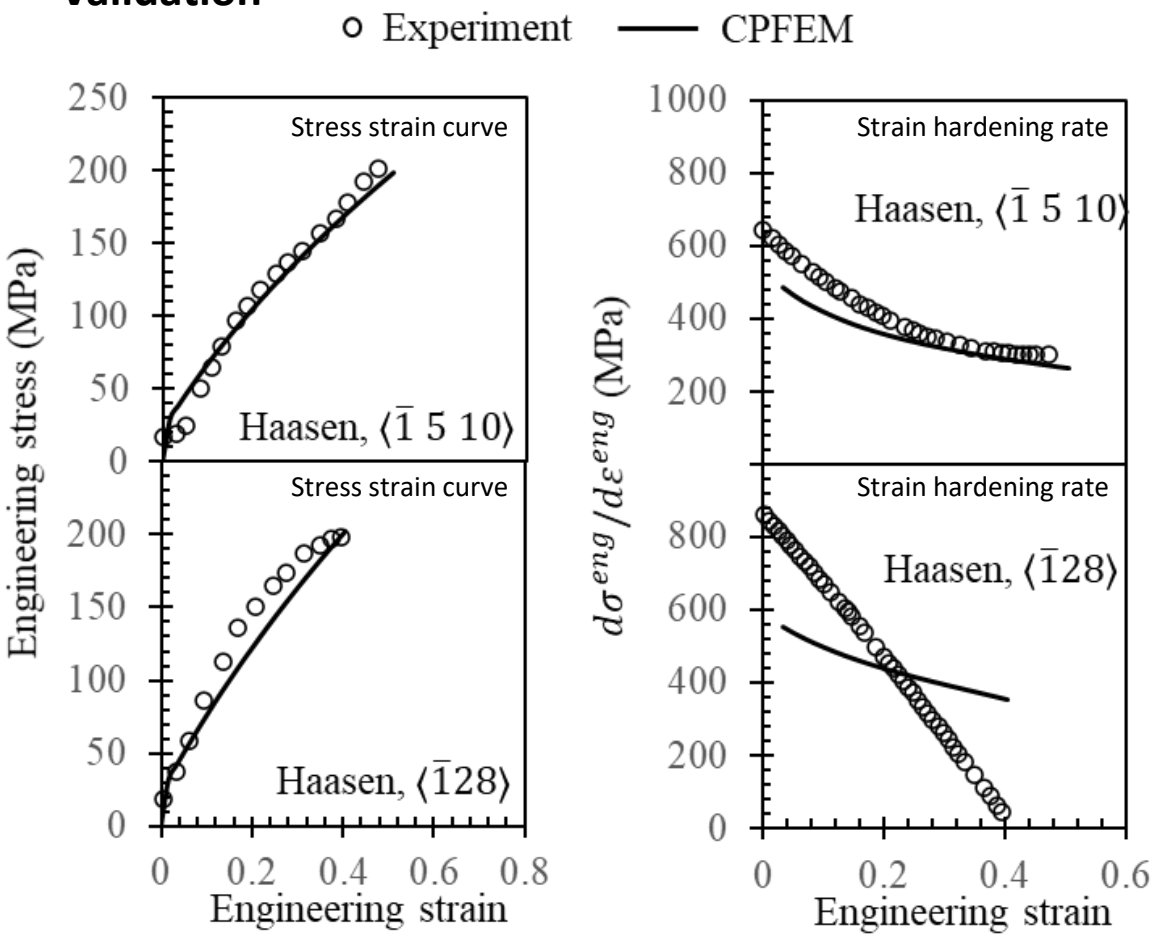
- CPFEM model parameters were calibrated from DFT-based predictions (except for the weighting parameter w)
- FEA using the calibrated CPFEM model agreed well with macroscale experiments

Calibration of w

Flat tensile specimen
$(2.5 \times 5.5 \times 0.25\ mm^3)$



Validation



Round wire specimen
Diameter = 2.24 mm
Length = 71.12 mm

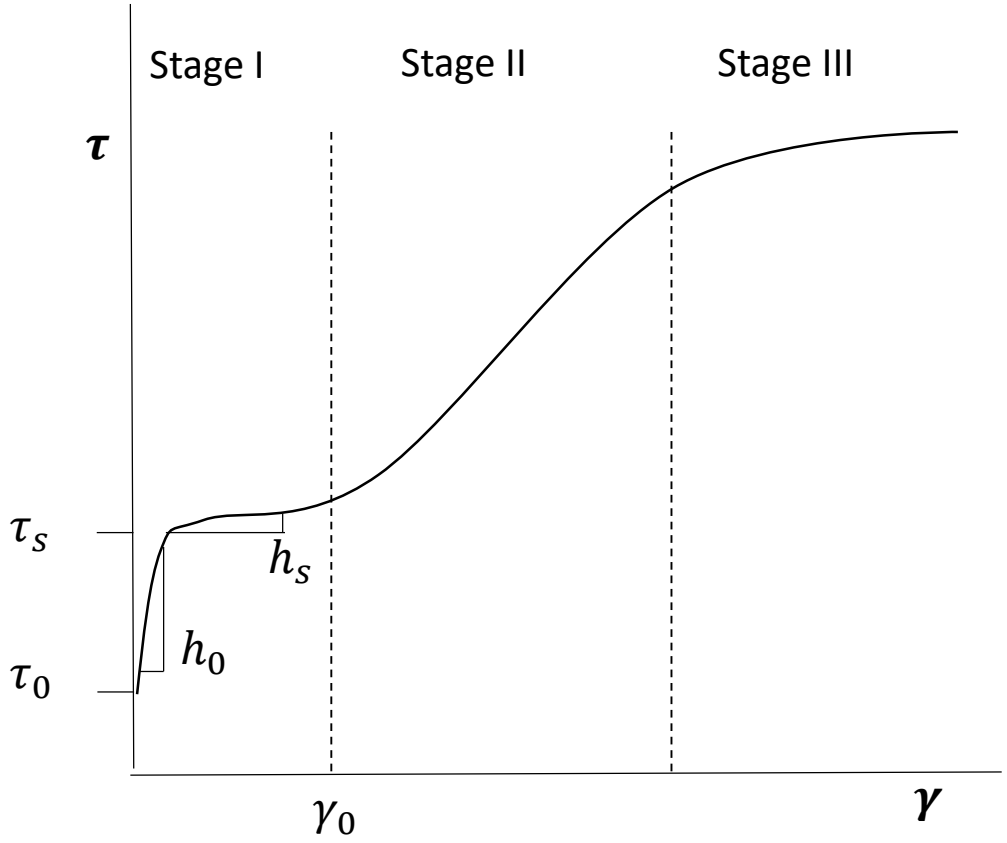
P. Haasen, *Philos. Mag.*, 1958.
Z. Yao et al., *J. Nucl. Mater.*, 2003.
S. Qin et al., *arXiv preprint arXiv, 2020.*

Polycrystals: Bassani-Wu modification to single crystal model

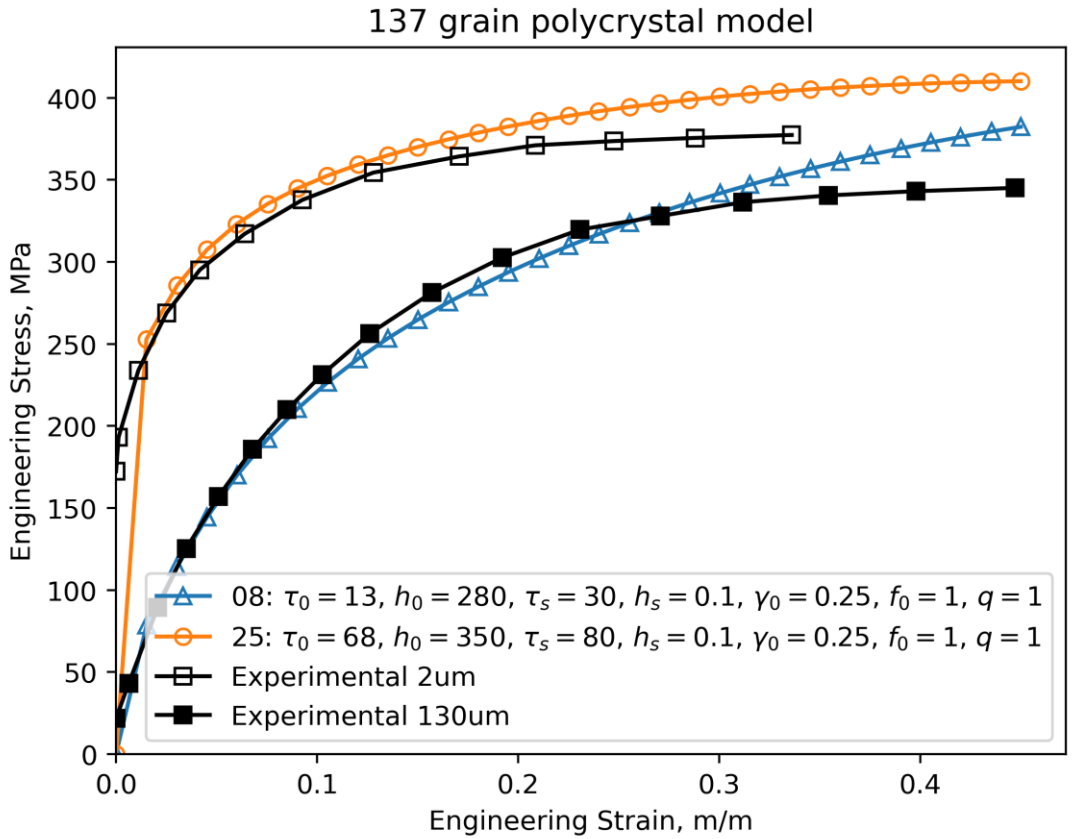
$$h_{\alpha\beta} = \{q - (q+1)\delta_{\alpha\beta}\} \cdot \left\{(h_0 - h_s)\,\mathrm{sech}^2\left[\frac{(h_0 - h_s)\gamma}{\tau_s - \tau_0}\right] + h_s\right\} \cdot \left\{1 + \sum_{\beta \neq \alpha} f_{\alpha\beta} \tanh\left(\frac{\gamma^\beta}{\gamma_0}\right)\right\}$$

*Extra parameters from Bassani-Wu model in red

Single slip system behavior:

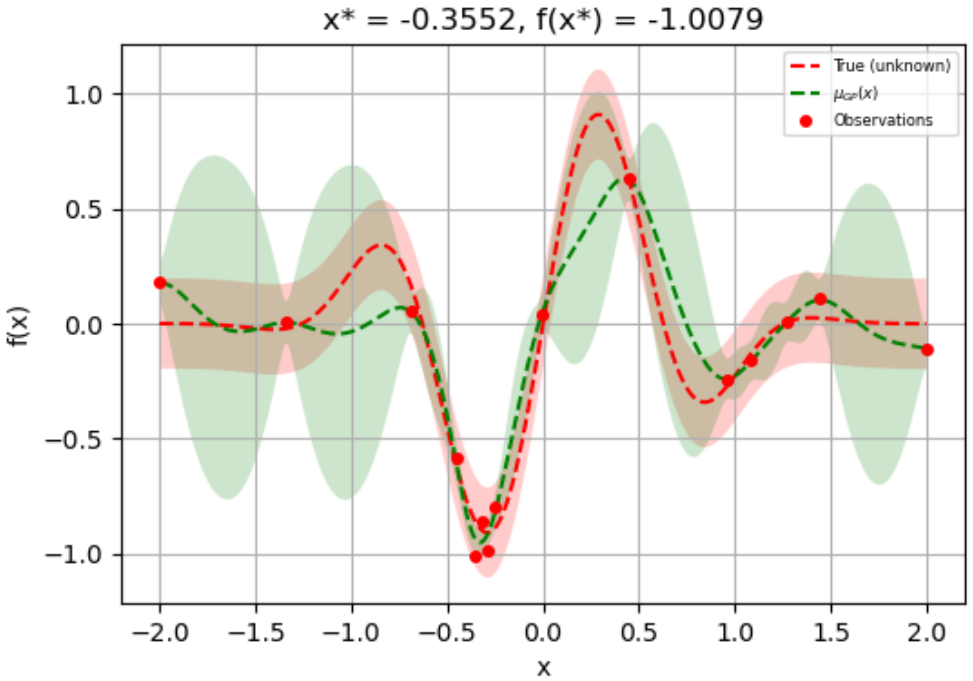


Polycrystal behavior:



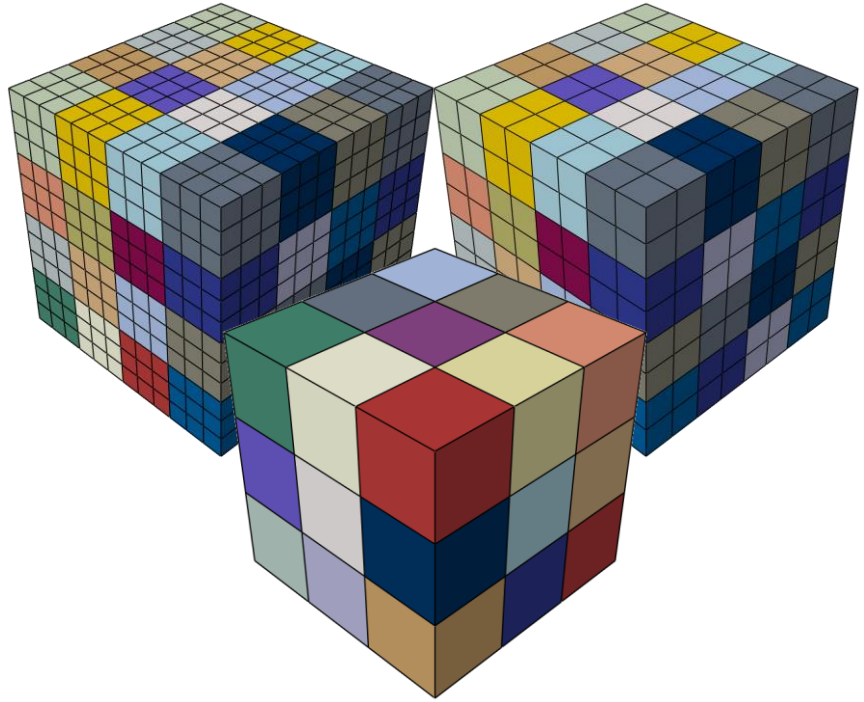
Polycrystals: Automated optimization

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

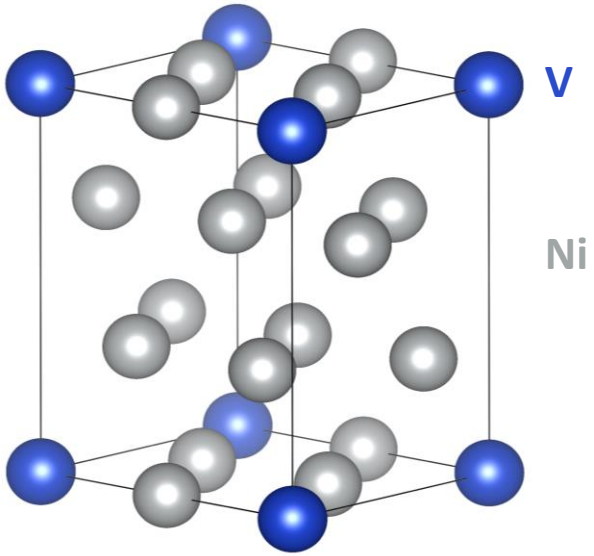
Simplified polycrystal microstructures:

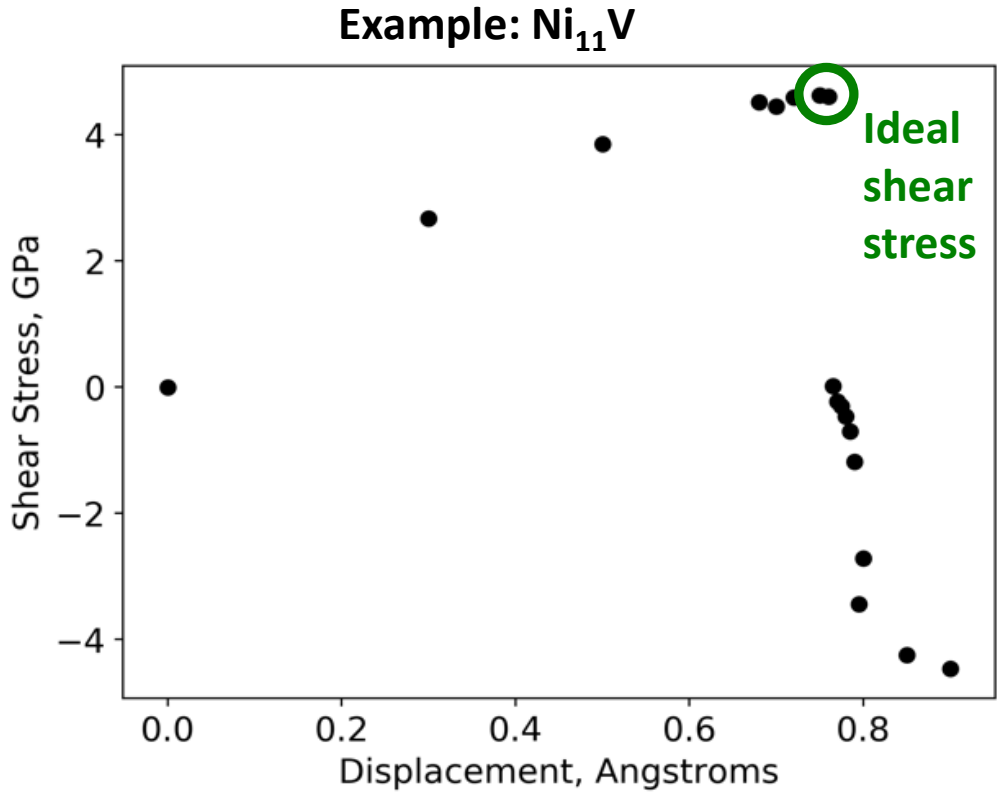


Used to find optimal Bassani-Wu parameters that match **experimental data** for polycrystal nickel of different **grain sizes**

Alloys: Ideal shear strength of Ni-X ($Ni_{11}X$)

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

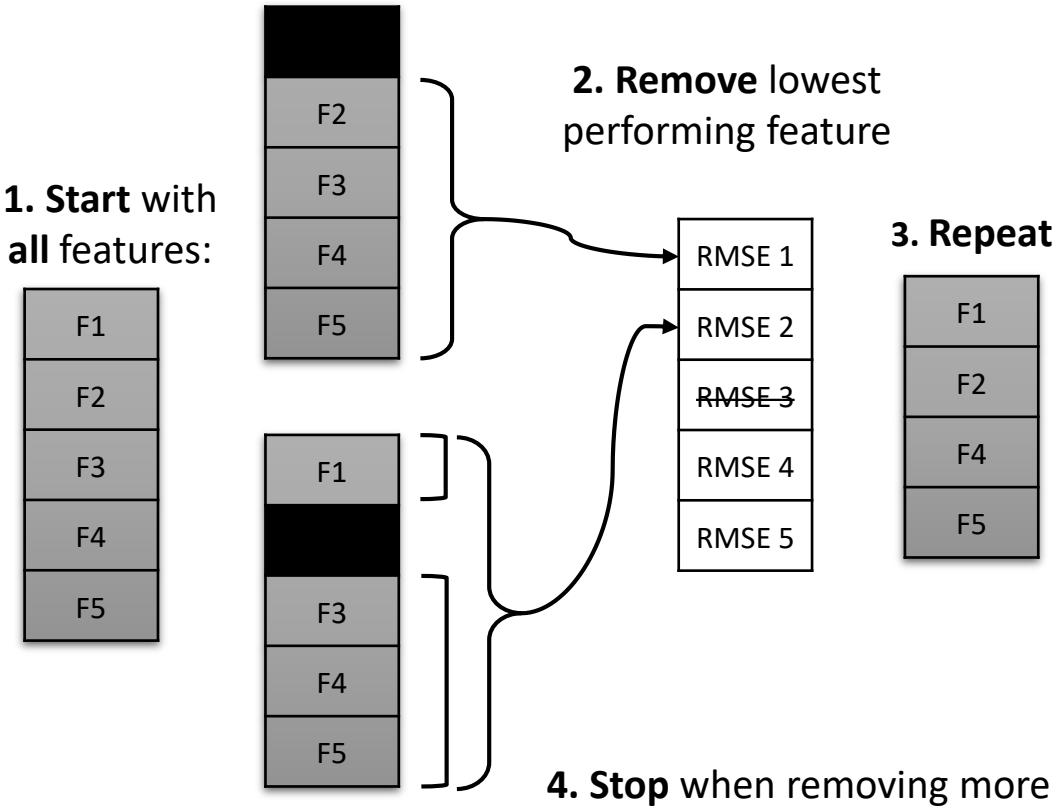




Alloys: Sequential wrapper method, correlations

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:

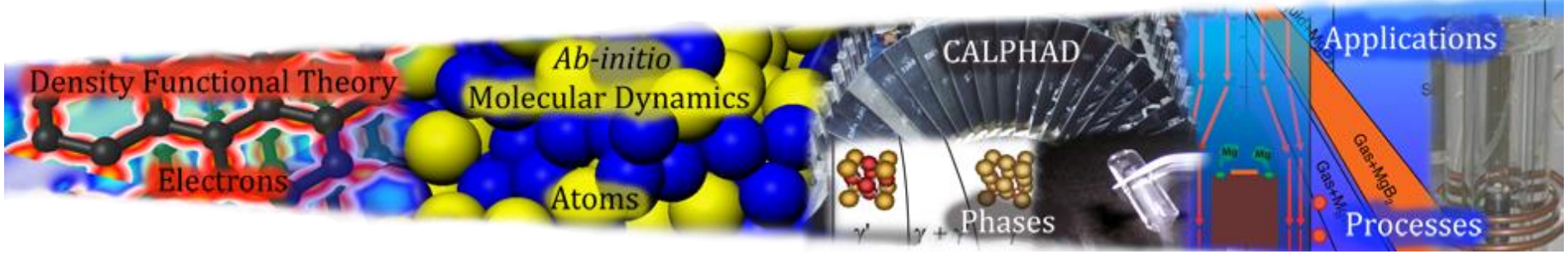


Forward variant: add features whose addition results in the lowest RMSE

Index	Ftest	rRelief	R^2	MIC	wrapper-backward	wrapper-forward
1	Radius_ Coval	V0_Zhang	V0_Zhang	V0_Zhang	Ele_Conduc	V0_Zhang
2	NdUnfill	EleDensity_ Zhang	EleNeg_ Zhang	EleNeg_ Zhang	V0_Zhang	DebyeT
3	EleNeg_ Pauling	M_Num2	EleDensity_ Zhang	DebyeT	NfVal	G_wiki
4	NdVal	Radius_ Coval	Radius_ Coval	Y_wiki	DebyeT	Ele_Conduc
5	V0_Zhang	S298	DebyeT	G_wiki	Heat_ capacity	NfUnfill
6	Group	EleNeg_ Zhang	EleNeg_ Pauling	M_Num2	EleDensity_ Zhang	Y_wiki
7	EleNeg_ Zhang	PP_ radius_s	M_Num2	Radius_ Coval	Radius_ Coval	EleNeg_ Zhang
8	NUnfill	PP_ radius_p	G_wiki	EleDensity_ Zhang	Nval	Heat_ Sublimation
9	PP_ radius_p	Max_range _electrons_ in_solids	Y_wiki	NdUnfill	NpVal	B_wiki
10	M_Num2	DebyeT	NUnfill	Group	Mass	BoilingT

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 $\Rightarrow$ Ideal shear strength of Ni and $Ni_{11}X$ by DFT calculations and machine learning understanding