High Throughput Computational Framework of Materials Properties for Extreme Environments

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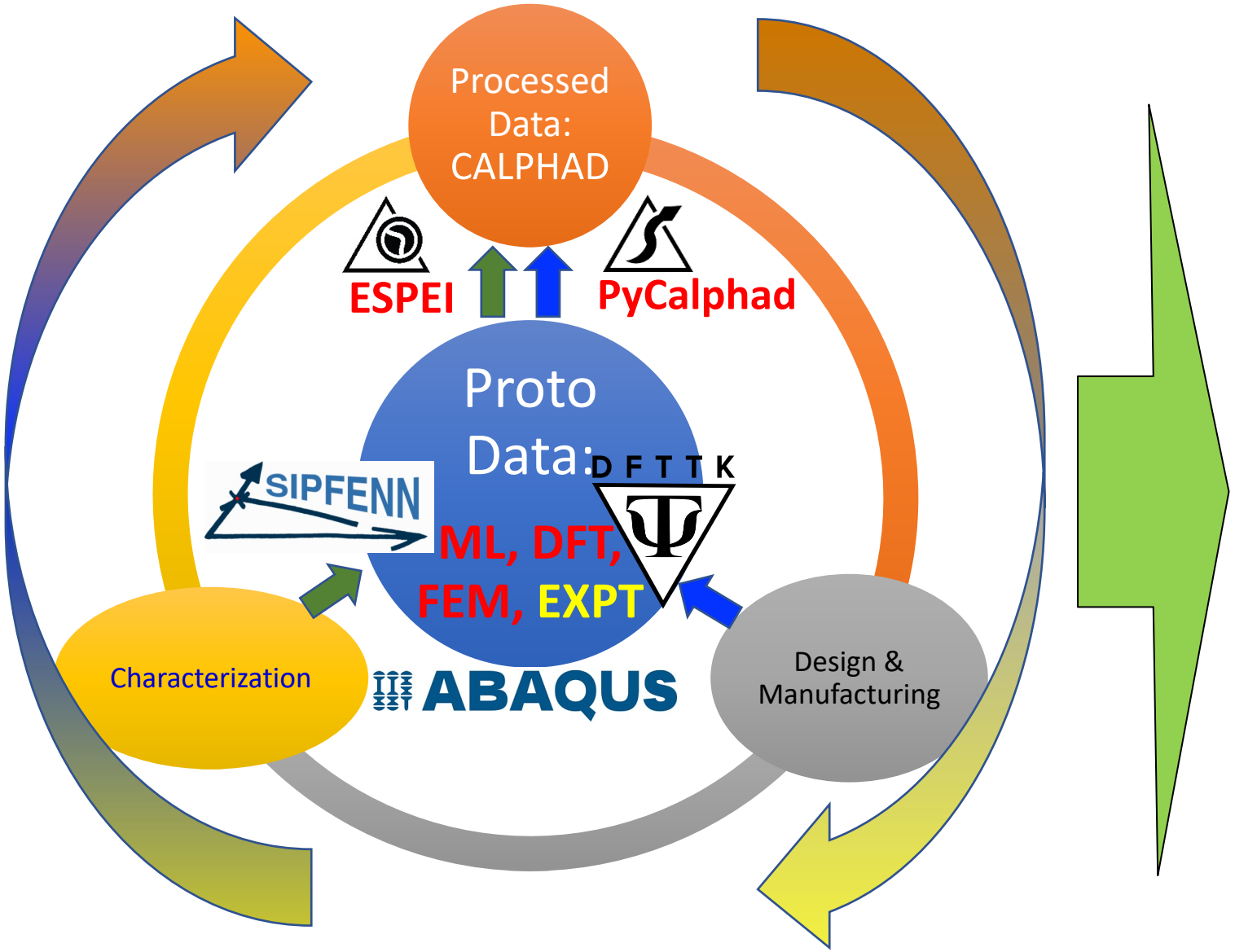
Outline

- 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

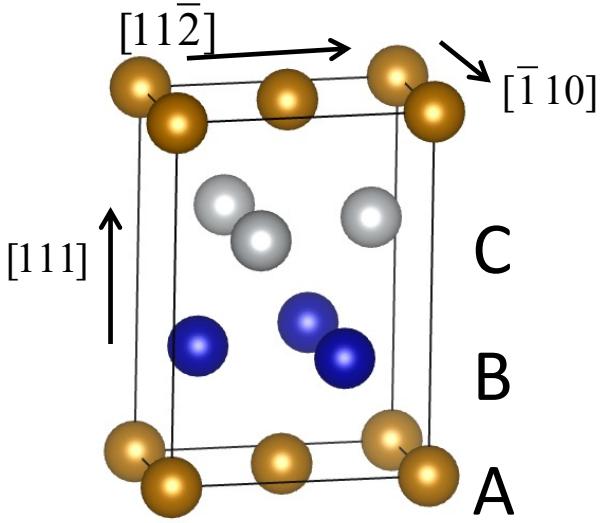


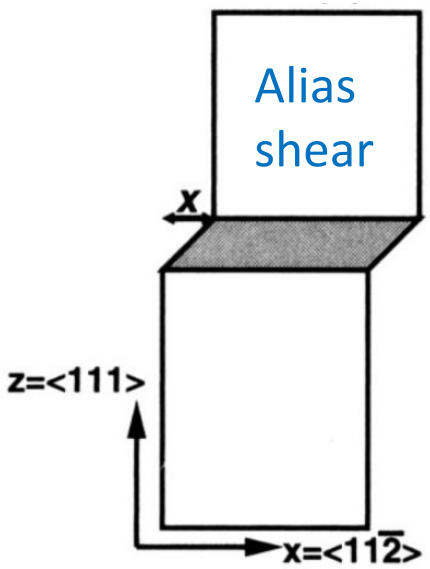
- ✓ Predict proto data using DFT Tool Kit (www.DFTTK.org) and machine learning models (https://phaseslab.com/sipfenn/)
- ✓ Apply FEM (ABAQUS) to predict tensile strain-stress curve
- ✓ Use CALPHAD approach (PyCalphad.org and ESPEI.org) to model processed data
- ✓ Validate results and improve models

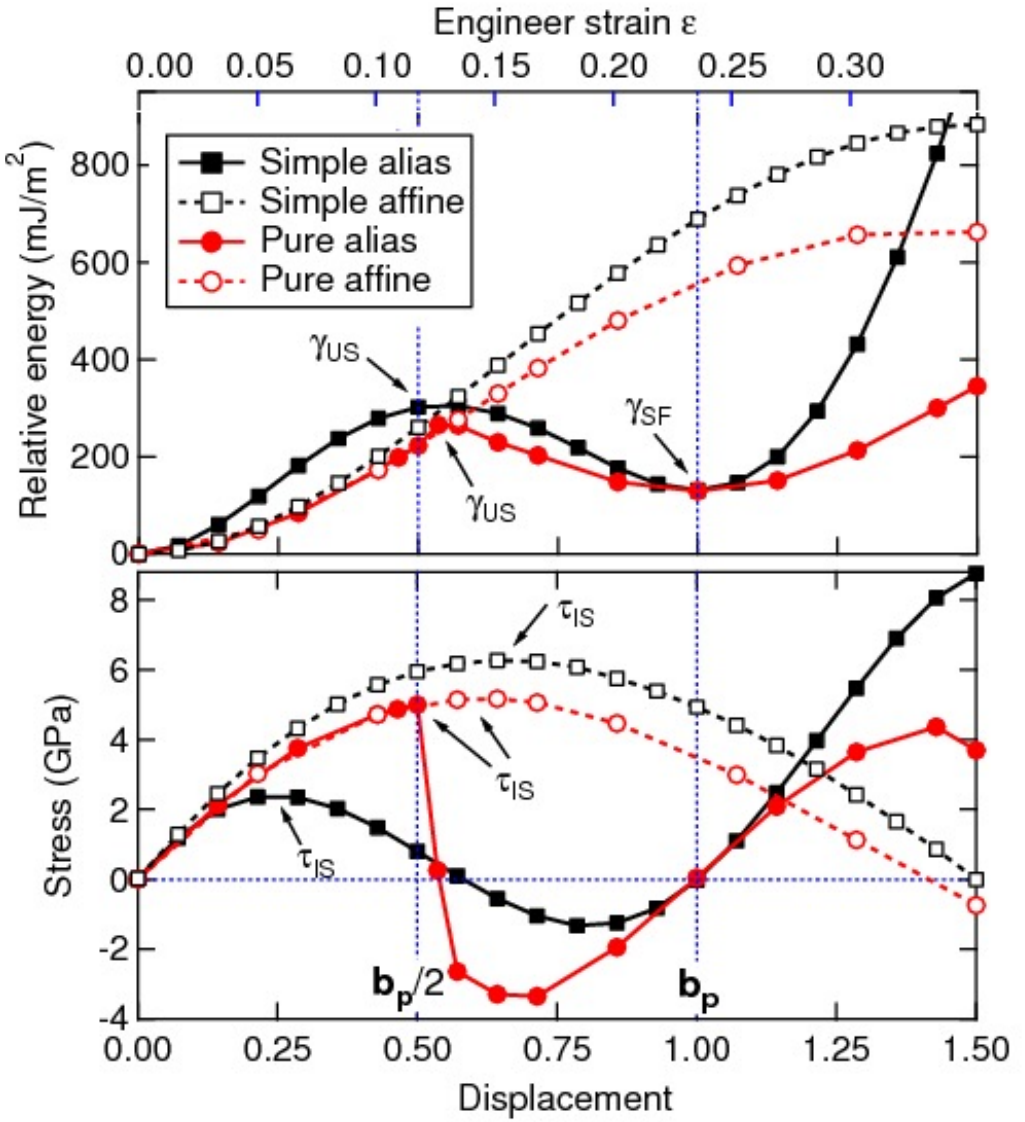
DFT calculations of *generalized stacking fault energy*

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

γ_{SF}: Stacking fault energy
γ_{US}: Unstable stacking fault energy
τ_{IS}: Ideal shear strength







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Ideal shear strength of pure elements (GPa)

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

Elems	60
bcc	18
fcc	45
hcp	50

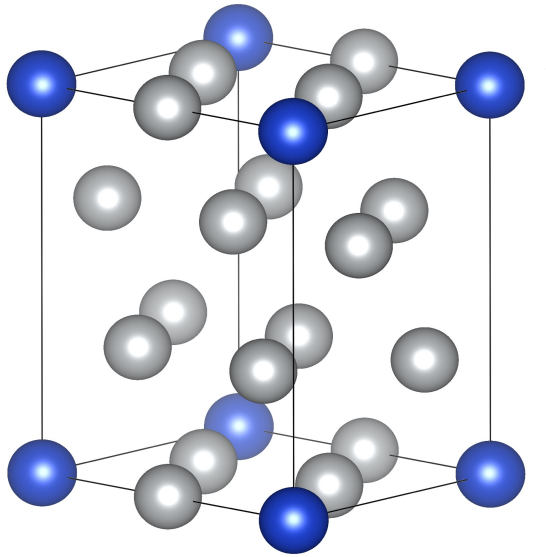
(Diamond: C, Si, Ge)

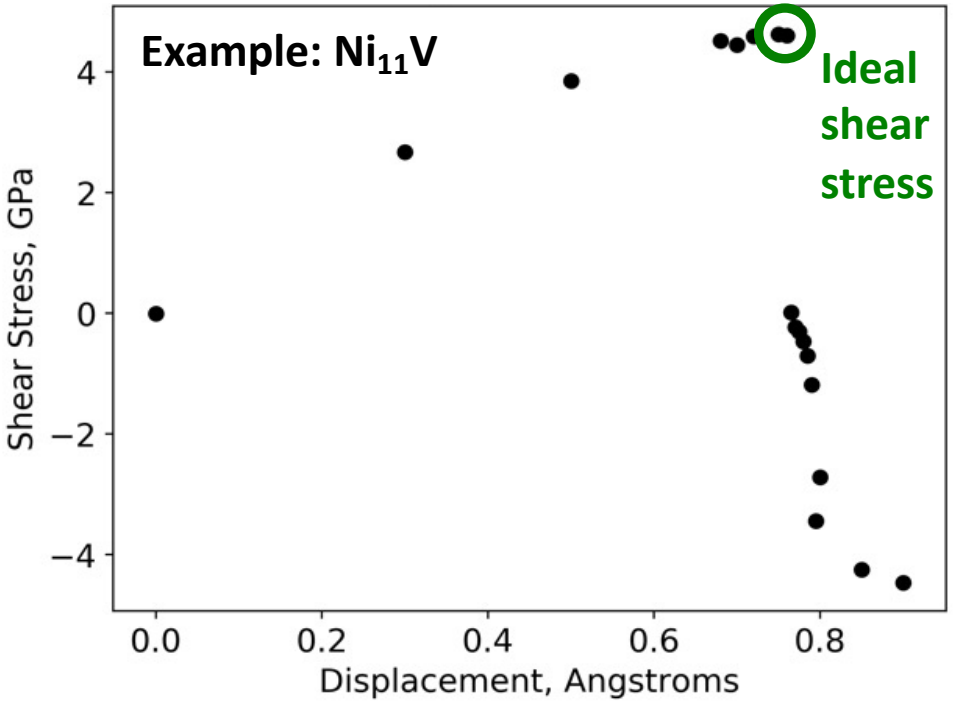
Li 3	Be 4												C 6 (79.9)
0.20	14.00												
0.15	5.22												
0.40	15.09												
Na 11	**Mg 12**											**Al 13**	**Si 14 (7.2)**
0.44													
0.09	0.61											2.66	
0.19	**1.50**												8.07
K 19	**Ca 20**	**Sc 21**	**Ti 22**	**V 23**	**Cr 24**	**Mn 25**	**Fe 26**	**Co 27**	**Ni 28**	**Cu 29**	**Zn 30**		**Ge 32 (5.0)**
0.11				5.16	19.01		7.56						
0.05	0.22	1.26	1.78			5.88	10.12	4.95	5.39	2.33			
0.09	0.42	2.81	4.39			6.05	11.34	6.55	3.56	2.42	2.18		4.01
Rb 37	**Sr 38**	**Y 39**	**Zr 40**	**Nb 41**	**Mo 42**	**Tc 43**	**Ru 44**	**Rh 45**	**Pd 46**	**Ag 47**	**Cd 48**		
0.07	0.10			5.86	15.44								
0.01	0.11	1.49	1.37			7.70	14.26	10.47	1.84	1.27			
	0.29	2.18	2.38			7.17	15.88	5.57	0.88	1.58	0.50		
Cs 55	**Ba 56**	**La 57**	**Hf 72**	**Ta 73**	**W 74**	**Re 75**	**Os 76**	**Ir 77**	**Pt 78**	**Au 79**	**Hg 80**	**Tl 81**	**Pb 82**
0.03	0.35			5.30	16.97						0.21	0.84	
0.01	0.01	1.33	2.41			11.11	19.97	15.47	1.50	0.72			1.02
0.02	0.27	0.63	5.08			10.65	21.77	6.65		0.95	0.22	0.79	0.23

Ce 58	**Pr 59**	**Nd 60**	**Pm 61**	**Sm 62**	**Eu 63**	**Gd 64**	**Tb 65**	**Dy 66**	**Ho 67**	**Er 68**	**Tm 69**	**Yb 70**	**Lu 71**
					1.01								
1.27	1.35	1.48	1.60	1.68	1.73	1.78	1.80	1.82	1.82	1.85		0.26	
0.51	0.54	0.55	0.55	0.62	0.83	1.09	1.48	1.85	2.16	2.47	2.70	0.43	2.85

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

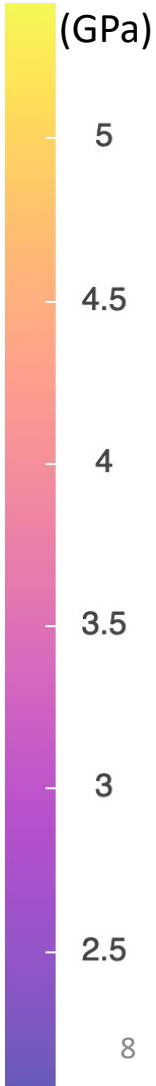
- Alias shear deformation to Ni-X ($Ni_{11}X$) solutio
- 26 alloying elements X
- Use alloying element **descriptors** to examine the variations of ideal shear strength





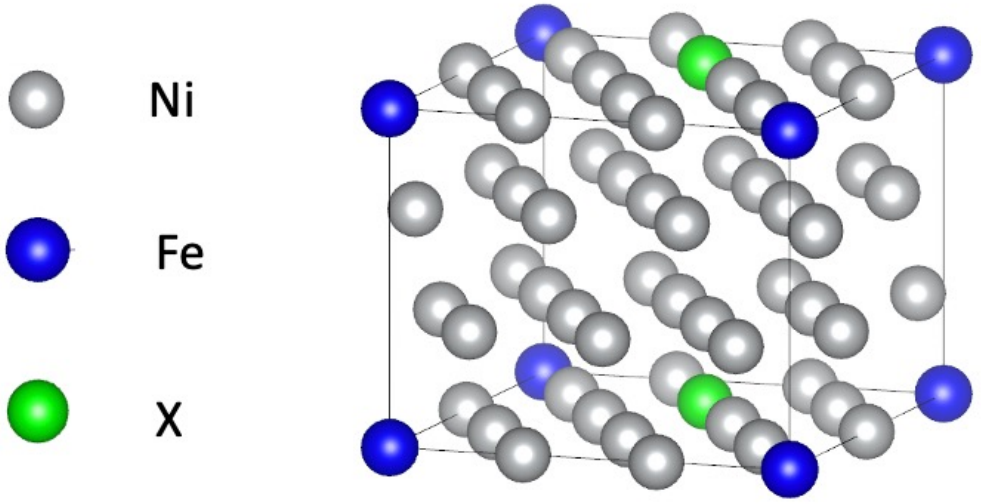
τ_{ideal}:

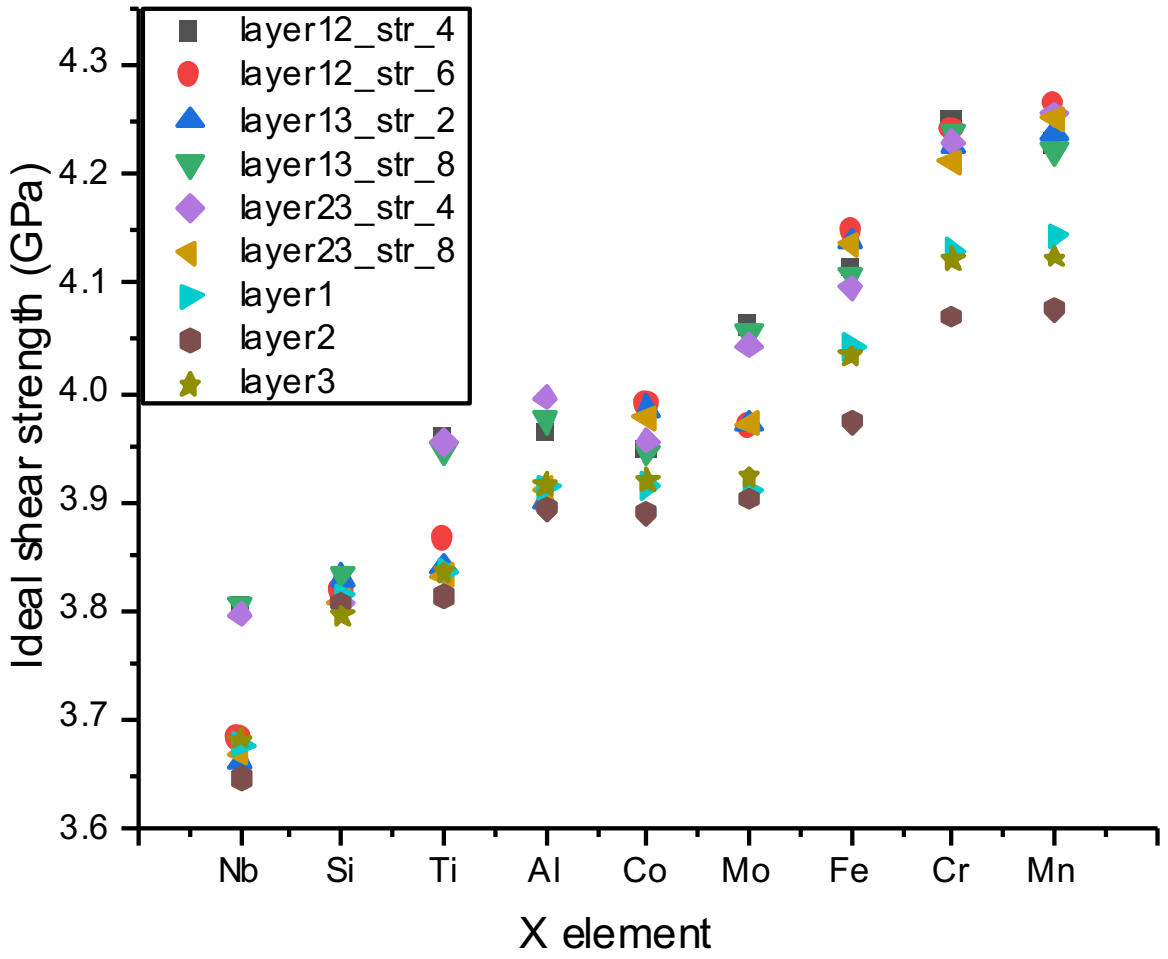
										13 Al	14 Si
21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge
39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn
71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb



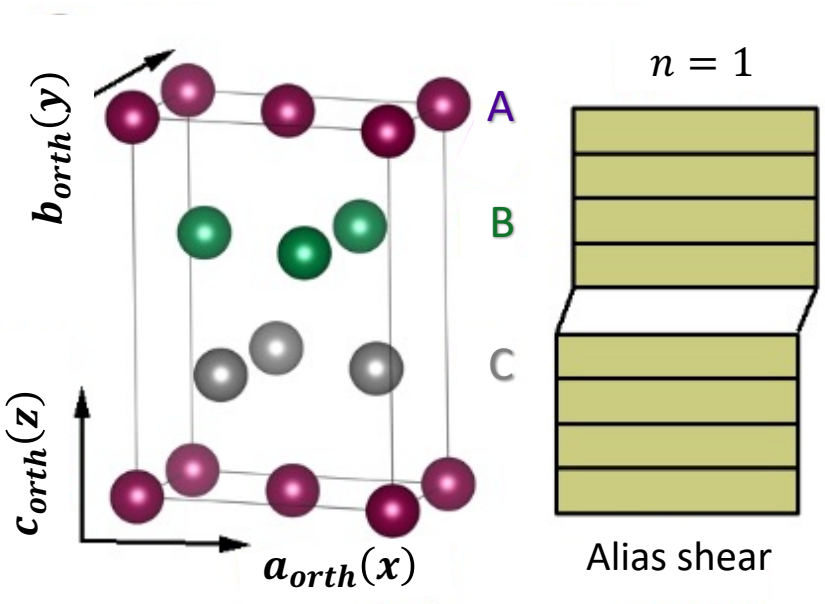
Ideal shear strength: Ternary Ni-Z-X ($Ni_{34}ZX$)

- Supercell: 36-atom with 3 {111} layers
- Total $Ni_{34}FeX$ configurations → 39
- 0.05 (Si) ~ 0.25 (Mn) GPa spread due to positions of Z and X in the supercell

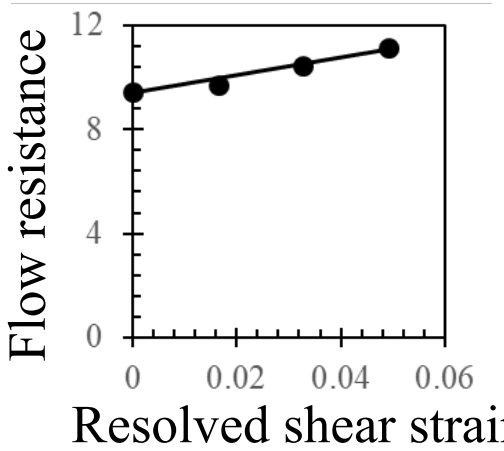


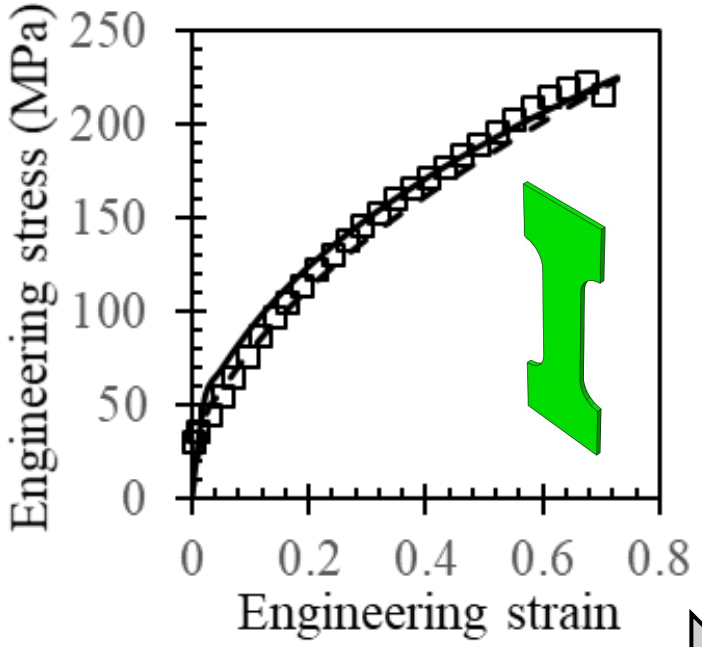


Multiscale predictive simulation: Single crystal



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





Atomic scale → Mesoscale → Macroscale

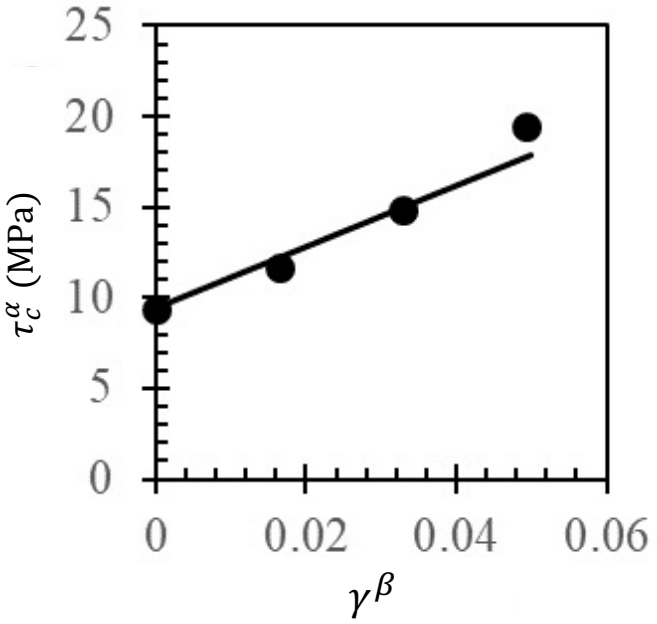
DFT-based predictions

Slip system hardening

Crystal plasticity

arXiv:2002.08552

Key contributions: Flow resistance

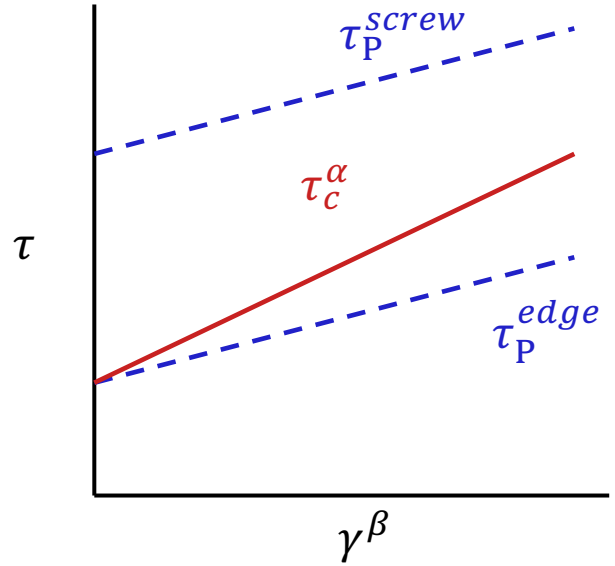


- Predicted by elastic properties and ideal shear strength based on the Peierls-Nabarro model
- At low strains: Edge dislocation

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

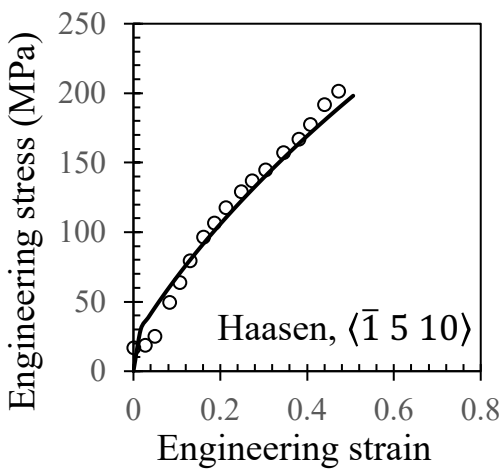
- At large strains: Junctions with screw components

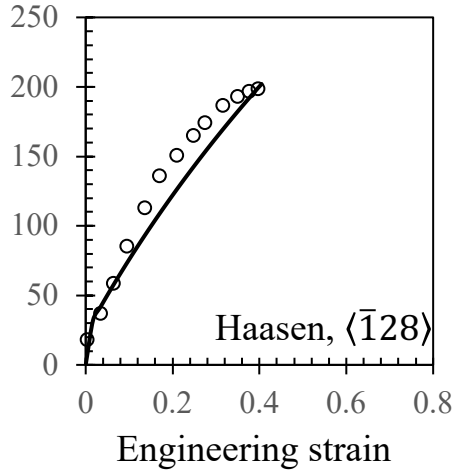
$$\tau_c^\alpha = \left(1 - w\gamma^\beta\right)\tau_{\mathrm{P}}^{edge} + w\gamma^\beta \tau_{\mathrm{P}}^{screw}$$

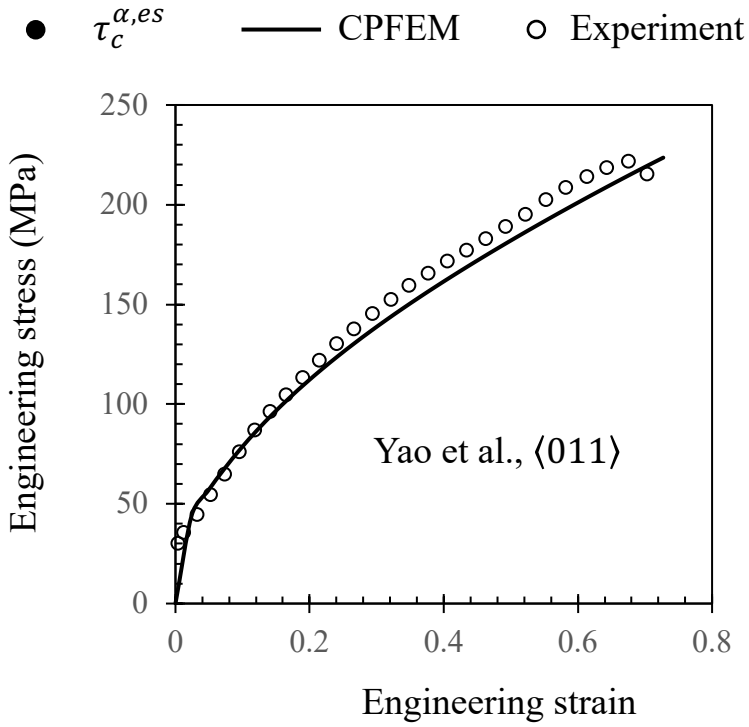


Stress-strain behavior of Ni: Single crystal

- $h_{\alpha\beta} = q_{\alpha\beta}\left[h_0 \operatorname{sech}^2\left|\frac{h_0\gamma}{\tau_s - \tau_0}\right|\right]$
  - τ_0 & h_0 from DFT predictions
  - w and τ_s calibrated to Yao data
- Predict large strain response of various orientations (Haasen data)

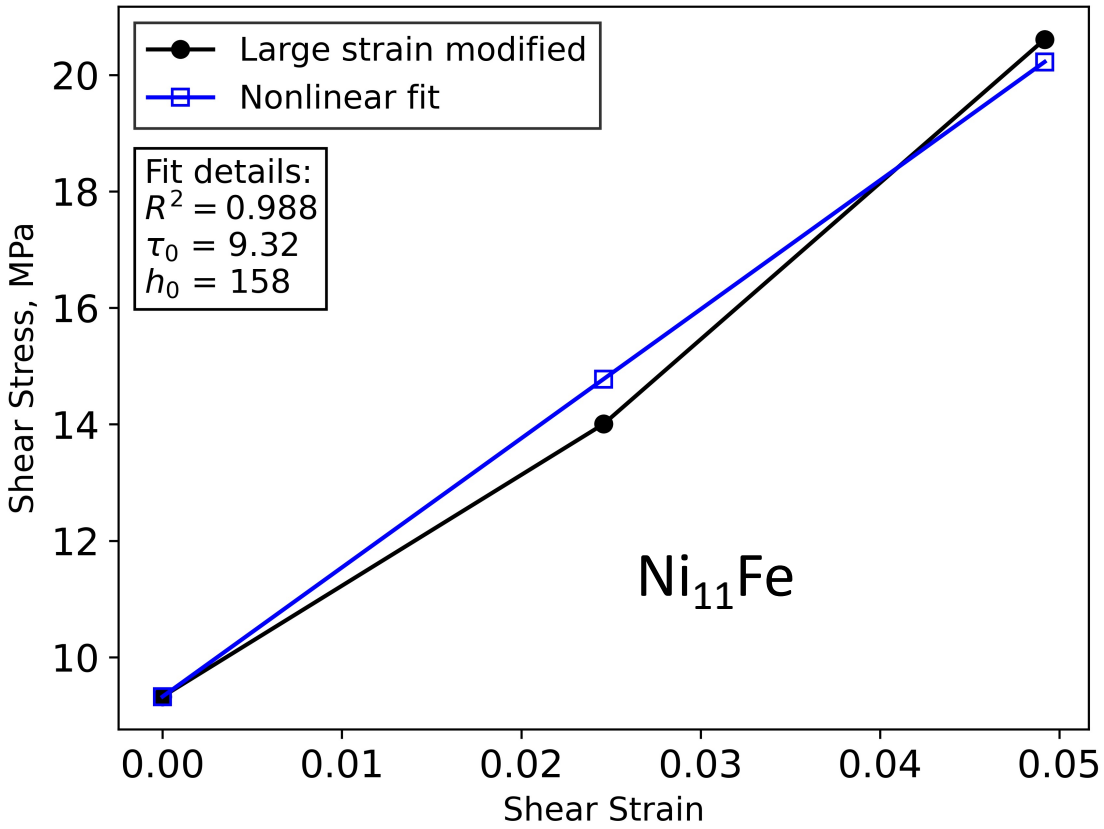




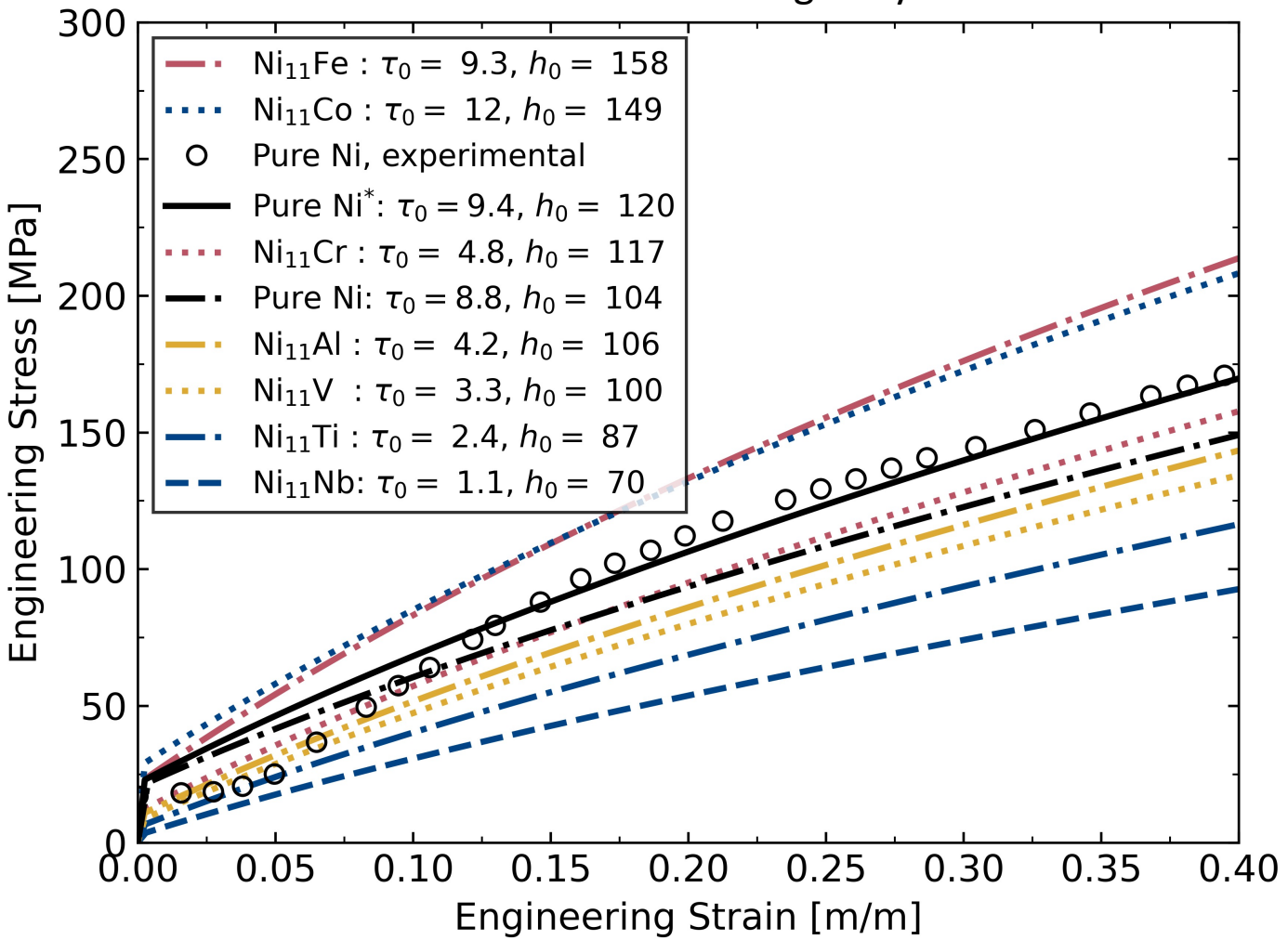


Haasen, *Philos. Mag. 1958,* 328, 384–418.
Yao et al., *J. Nucl. Mater. 2003,* 323:2–3, 388– 393.

Ni-X stress-strain behavior



Crystal plasticity finite element method results for single crystals

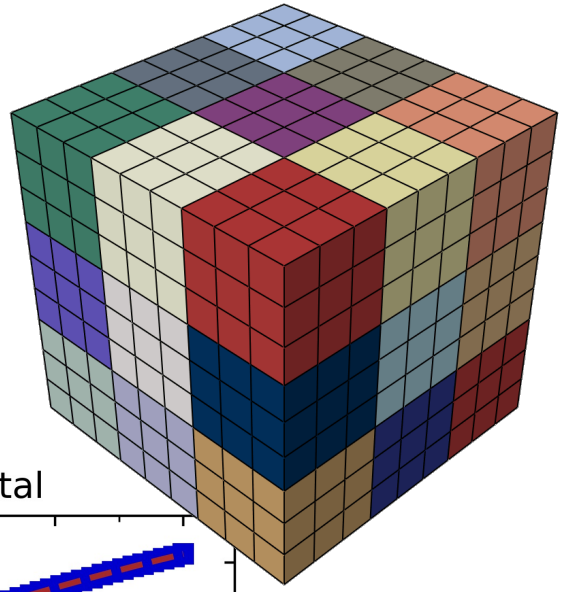


First-principles results considering pre-stra

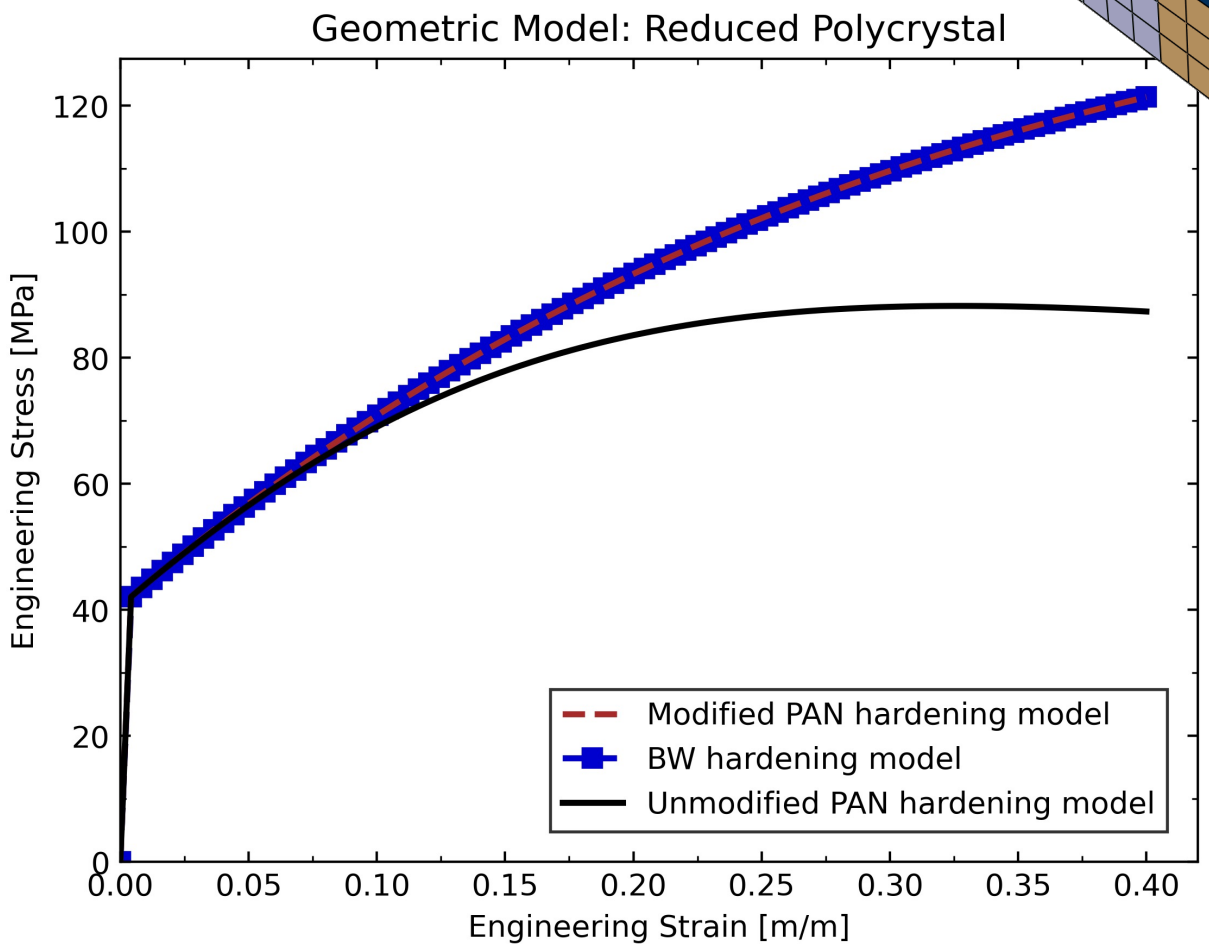
Resolved shear stress calculated using:

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

Polycrystal hardening moduli

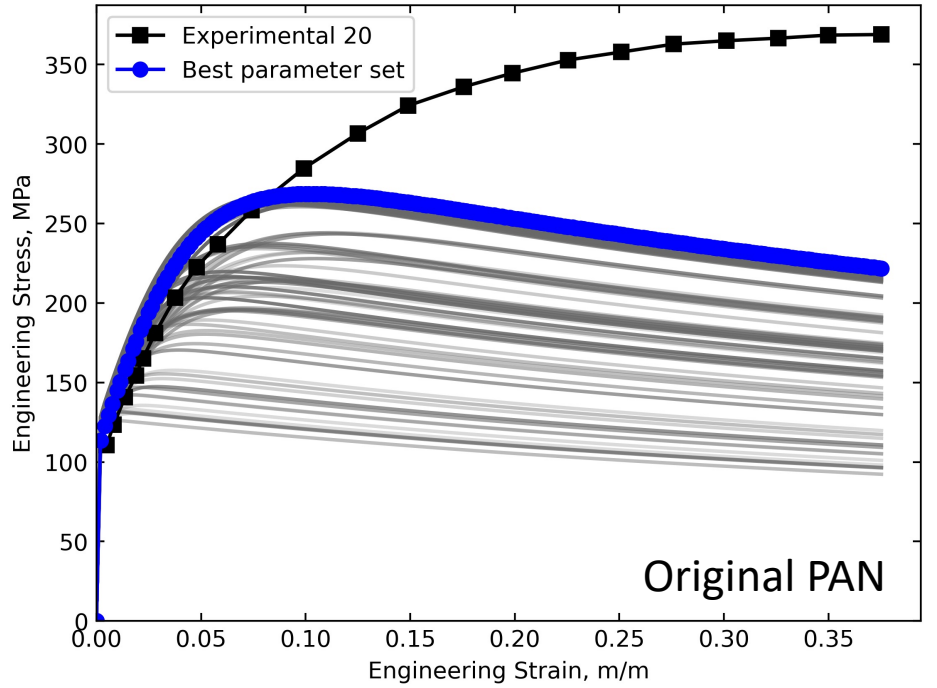


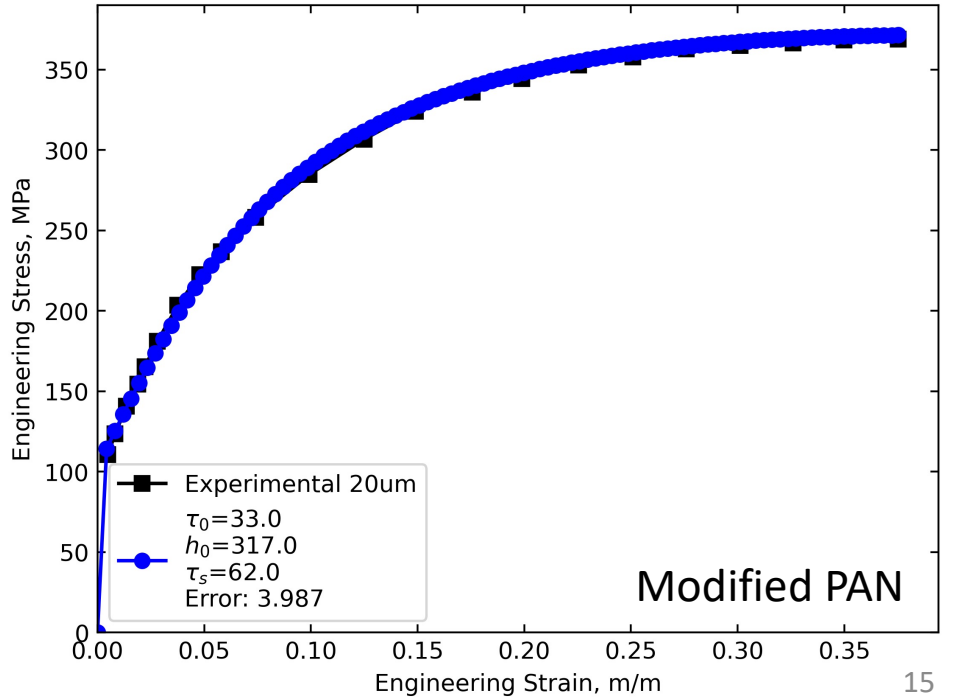
- Pierce-Asaro-Needleman
  - Function of $\gamma = \Sigma\gamma^{\beta}$
  - Three parameters: τ_0, h_0, τ_s
  - Limited hardening capacity
- Bassani-Wu
  - Function of γ^{β}
  - Two additional parameters
  - Higher hardening capacity
- Modified PAN
  - Function of γ^{β}
  - Three parameters
  - Higher hardening capacity



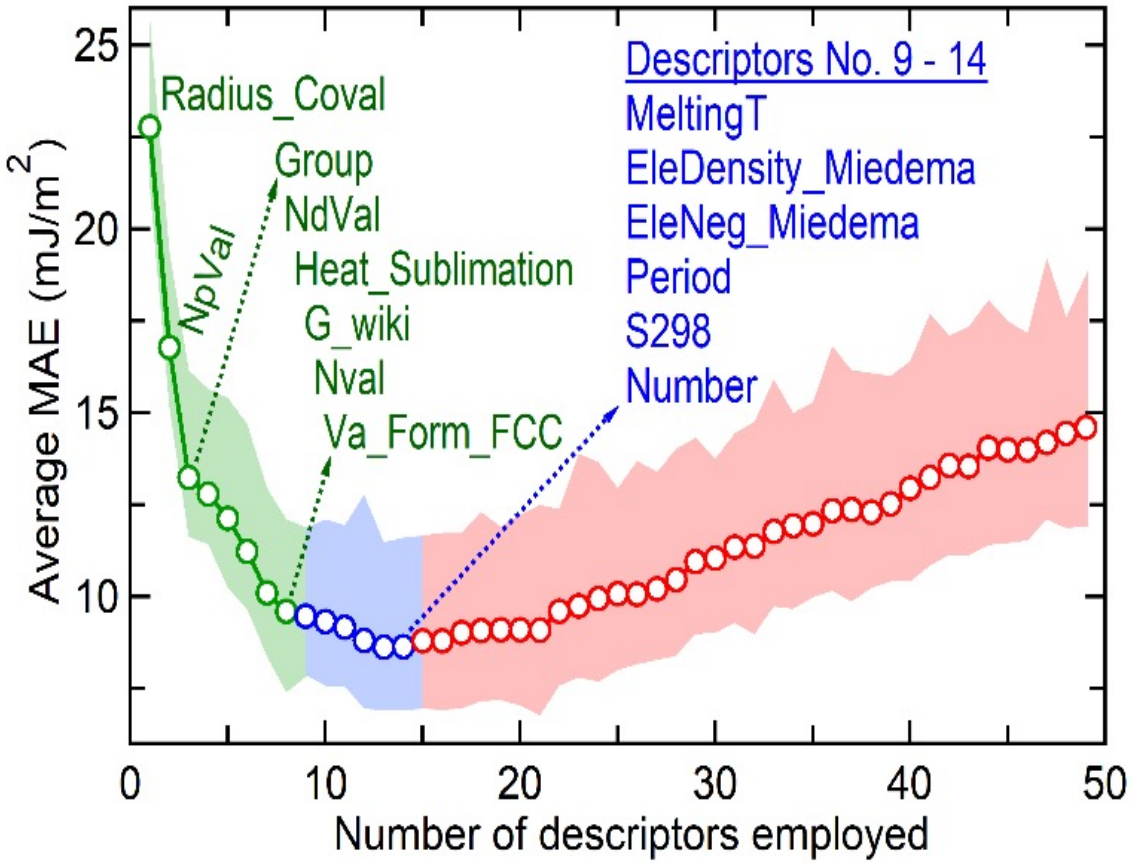
Polycrystal models

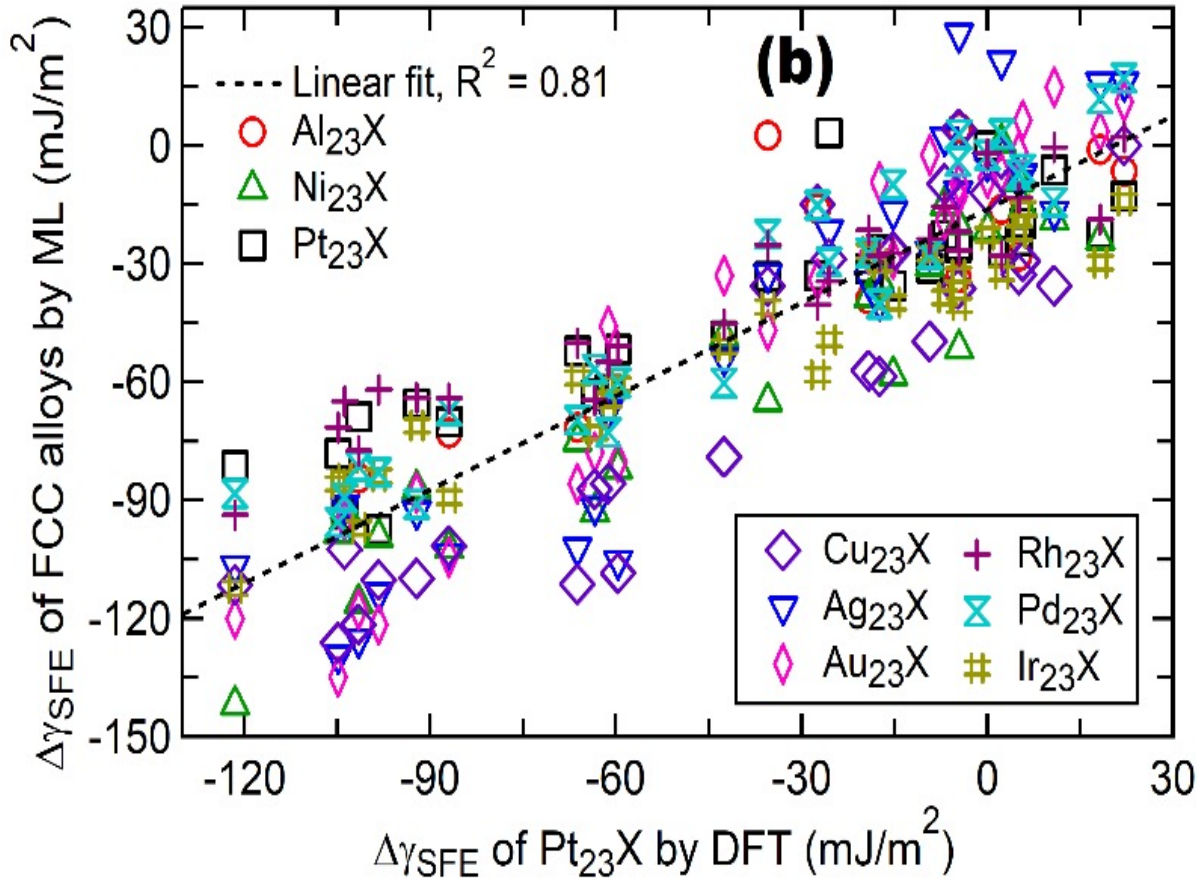
- Simplified polycrystal models
  - Accurate to larger microstructural models
  - Much more efficient
- Automated parameter search
  - Existing open-source optimization library, scikit-optimize (scikit-optimize.github.io)
  - No gradient information necessary (Bayesian optimization via Gaussian processes)
  - Independent of hardening model details
- Hardening model conclusions
  - PAN increased hardening capacity when using γ^{β}
  - Grain size dependence from literature on Ni, Cu





Correlation analysis of materials properties by machine learning: Stacking fault energy in dilute fcc-based alloys



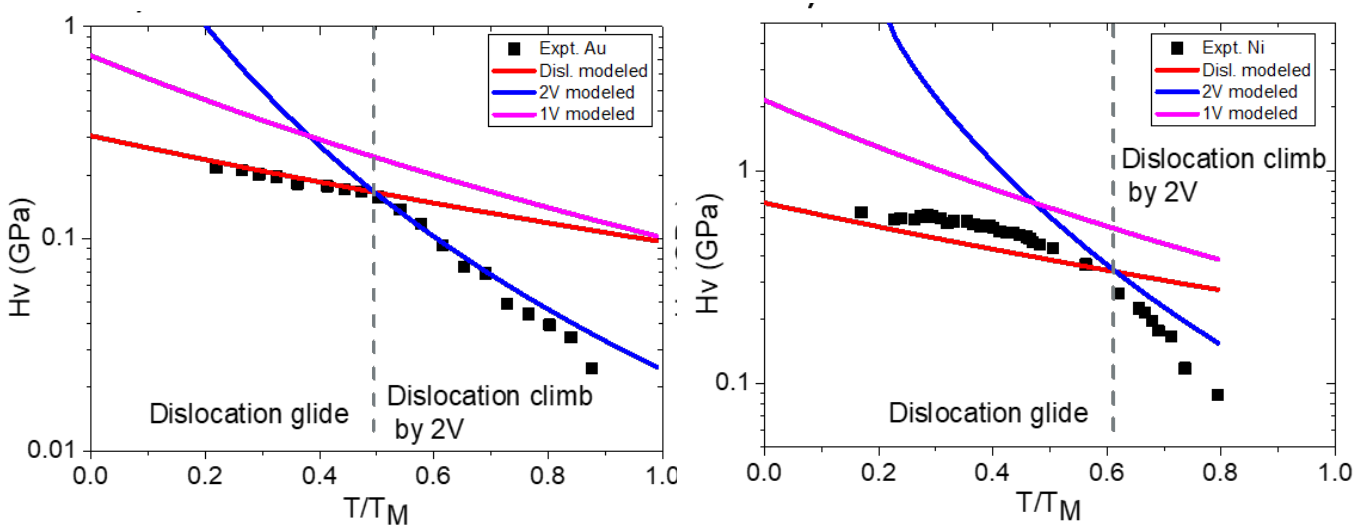


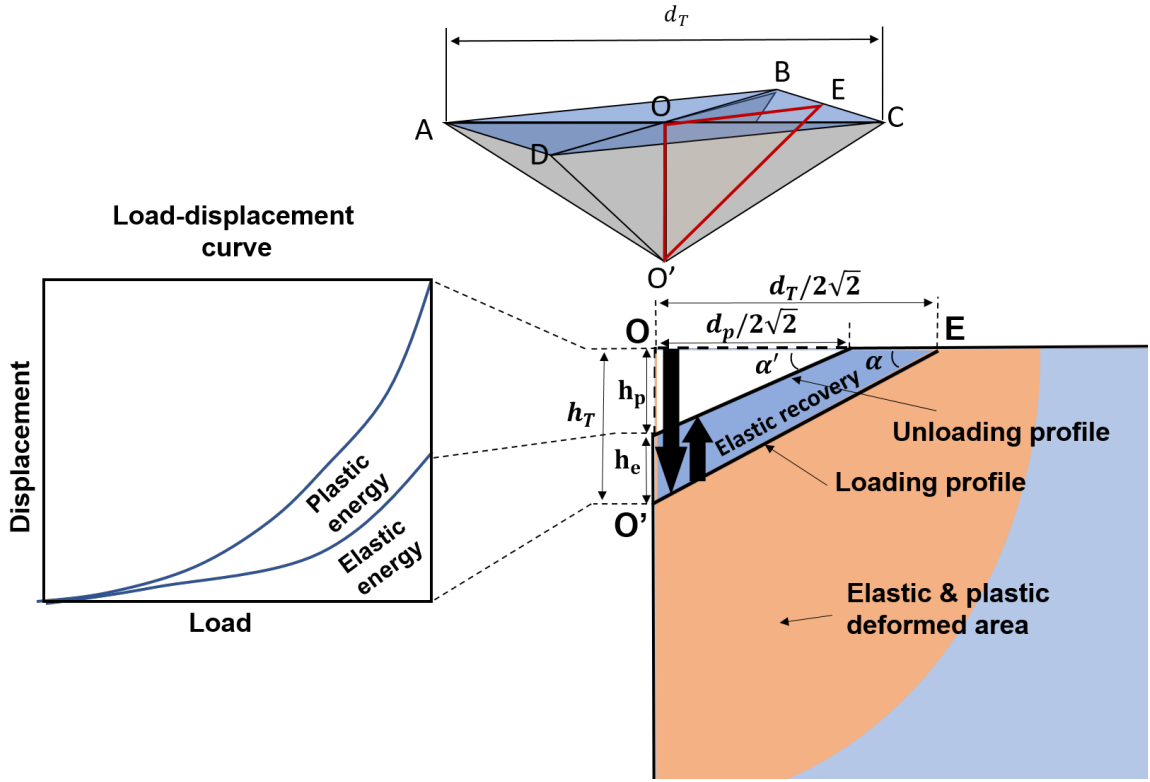
J Phys: Cond. Matter, 2021, DOI: 10.1088/1361-648X/ac0195

Temperature-dependent hardness model

$$H_v = 0.1615\,G\left(\left(1+5200\frac{b}{(1-v)^{2j}w(T)}\left(\frac{\tau_{PN}}{G}(T)\right)^2\right)^{\frac{1}{1.4}}\right)^2 e^{-2.2k}\left(\frac{b}{(1-v)^{j}w(T)}\right)^4 tan^{3/2}\alpha\,cos\,\alpha$$

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



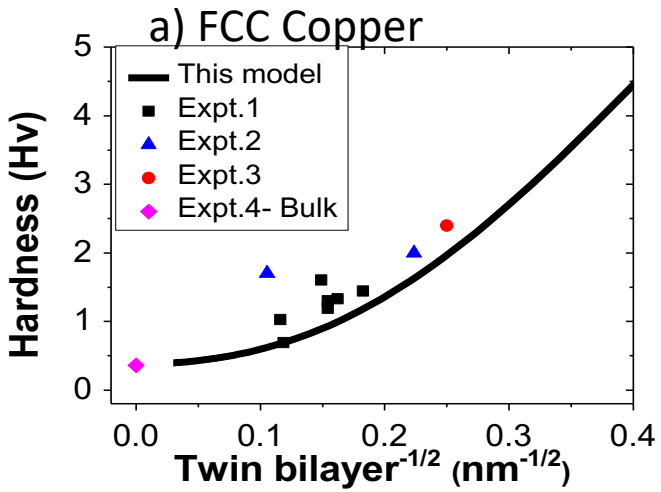


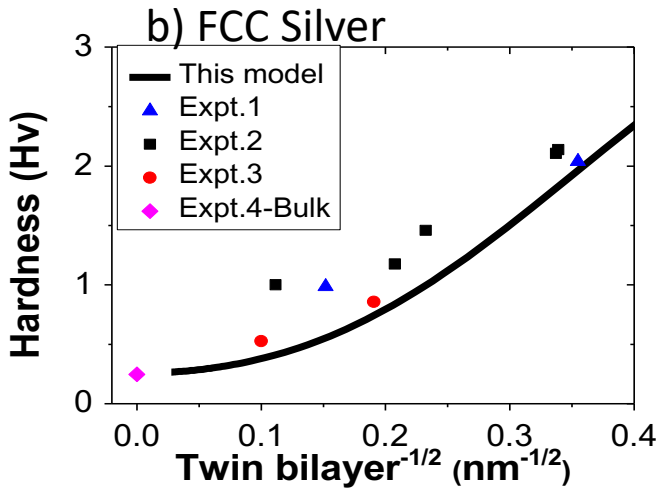
Hardness model for twin boundary

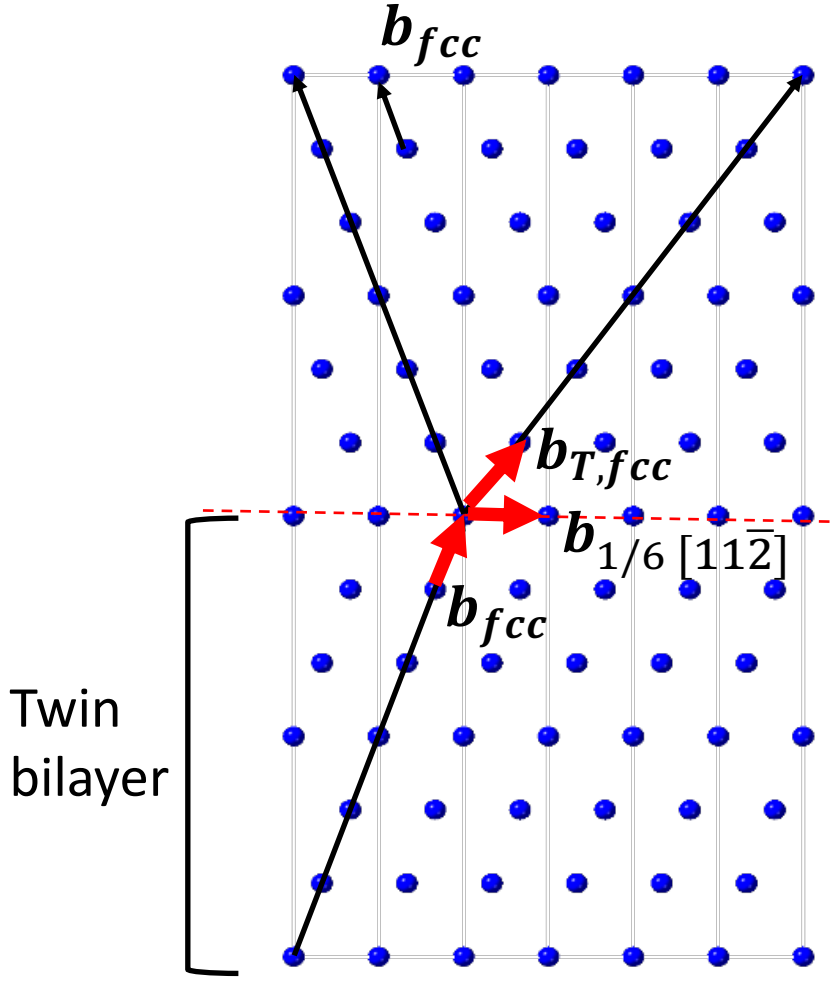
- For FCC metals:

$$b\left(\frac{1}{2}[110]\right) \rightarrow b_1\left(\frac{1}{2}[110]_T\right) + b_2\left(\frac{1}{6}[11\bar{2}]\right)$$

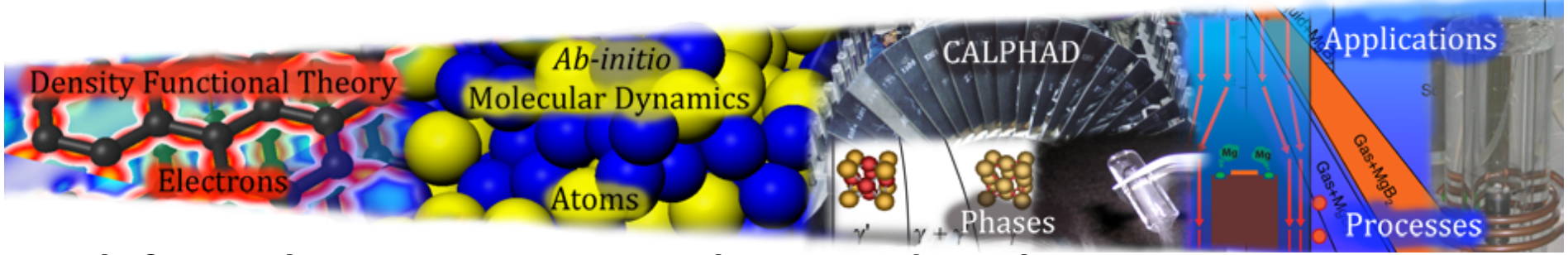
- Dislocation through twin boundary ➔ Shockley partial dislocations $\left(\frac{1}{6}[11\bar{2}]\right)$ activated near twin boundaries ➔ screw characteristics







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