SAND2021-14462C

An Fe-Ni-Cr-H Interatomic Potential and Hydrogen Effects on Stacking Fault Energies in Austenitic Stainless Steels

X. W. Zhou[1], C. Nowak[1], R. S. Skelton[1], M. E. Foster[1], J. A. Ronevich[1], C. San Marchi[1], and R. B. Sills[2]

[1]Sandia National Laboratories, USA; [2]Rutgers University, USA

2021 MRS Fall Meeting, Virtual, Dec 6 - Dec 8, 2021

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Stacking Fault Energy (SFE) on Hydrogen Embrittlement

- SFE is related to hydrogen compatibility parameter RRA (relative reduction in area) in JOM, 72, 1982 (2020):
  - RRA > 80% when SFE > 40 mJ/m^2;
  - RRA ~ 20-80% when SFE ~ 20-40 mJ/m^2.
- The austenitic stainless steels (e.g., 304L) deform through hydrogen-mediated slip bands in Metall. Mater. Trans. A, 52, 1516 (2021).
- We have performed a detailed study on SFE using molecular dynamics (MD). This has also led to an Fe-Ni-Cr-H potential.

Presentation Outline

- An Fe-Ni-Cr-H interatomic potential
- Experimental validation of molecular dynamics (MD) simulations
- Stacking fault energy calculations

The presented work has been published in Inter. J. Hydrogen Energy.

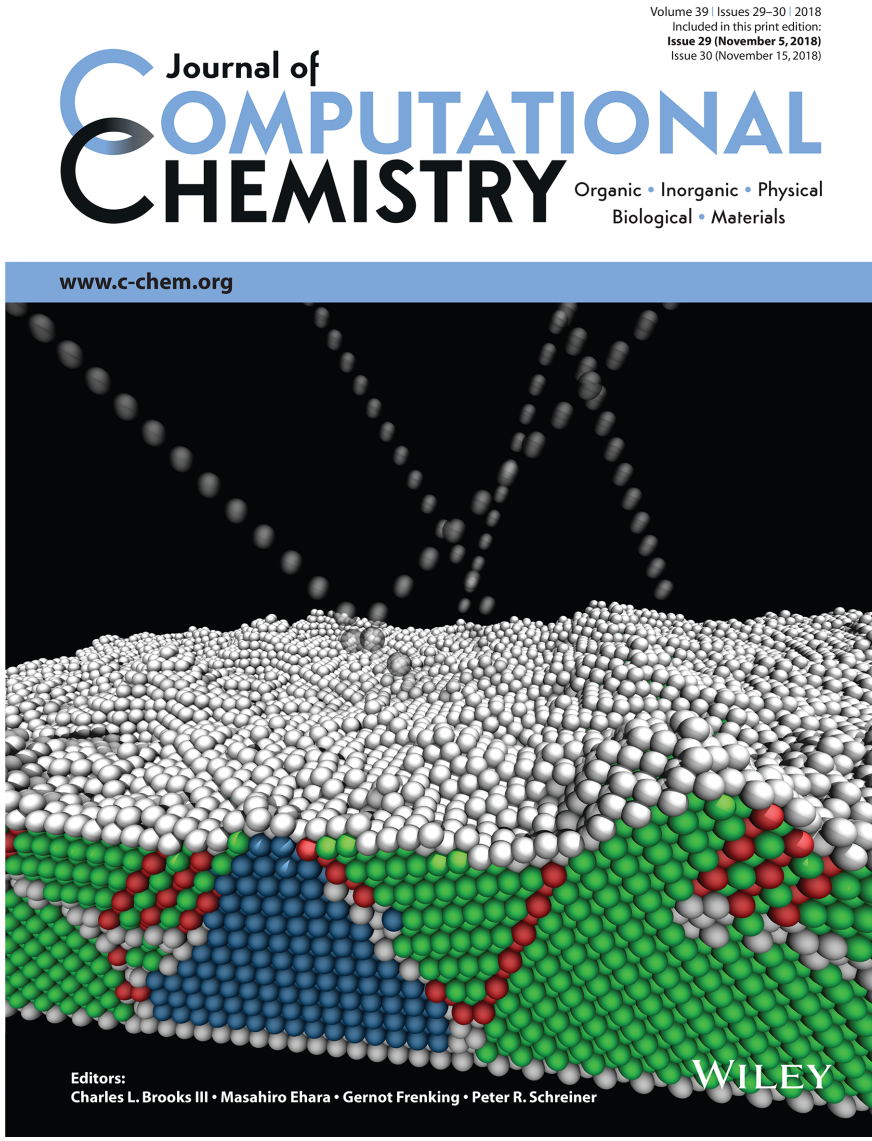
Adding H to an Existing Fe-Ni-Cr Potential

- No Fe-Ni-Cr-H potential is available in literature, but H can be added to an existing Fe-Ni-Cr potential.
- Smith and Was' potential (PRB 1989, 40, 10322) was fitted to effective atoms and did not consider SFE (stacking fault energy), not chosen.
- The 2013 Bonny et al's potential (MSMSE 2013, 21, 085004) predicts phase separation, not chosen.
- The 2011 Bonny et al's potential (MSMSE 2011, 19, 085008) predicts negative slope of SFE with Ni composition (should be positive), not chosen.
- Tong et al's potential (Mol. Sim. 2016, 42, 1256) predicts large negative stacking fault energy, not chosen.
- The 2018 Bonny et al's potential (MSMSE, 2018, 26, 065014) is based on the 2013 version, not chosen.
- We adopted our Fe-Ni-Cr potential (J. Comp. Chem., 2018, 39,2420).
- Other potentials (e.g., by Mendelev et al) are also available more recently, but are not tested.

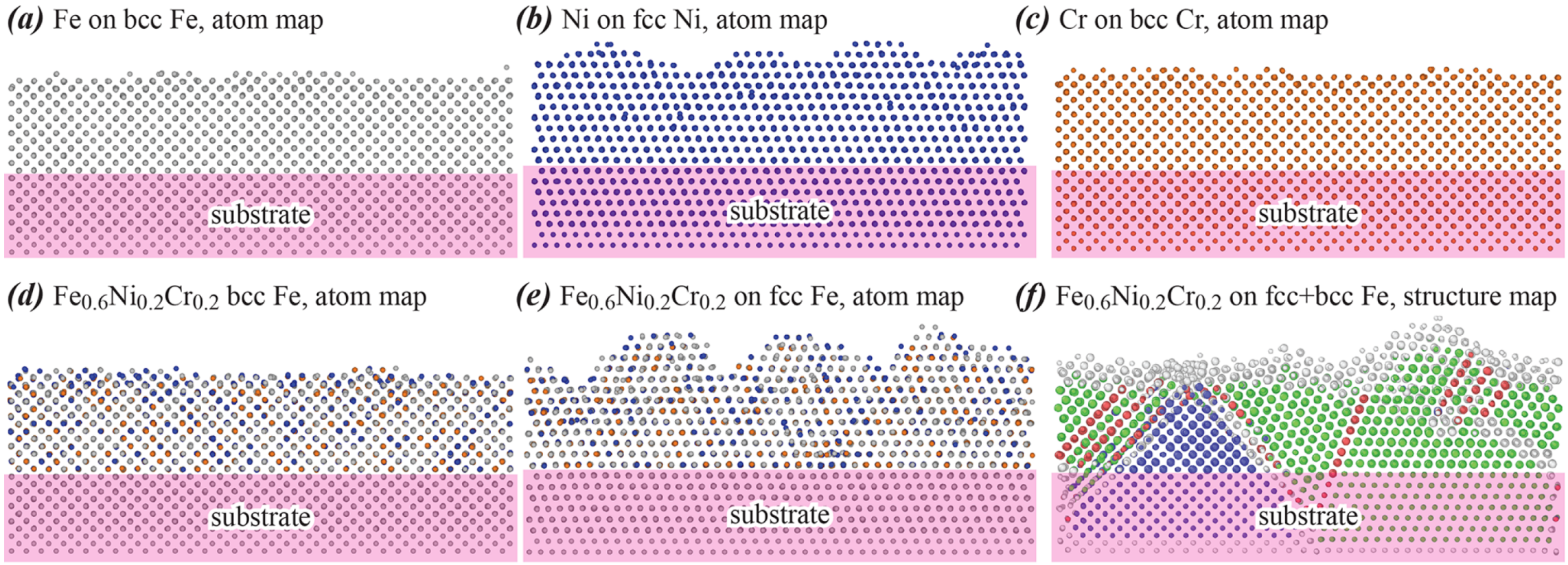
Our Fe-Ni-Cr-H Potential

- ❑ Energy, volume, stability trends in Fe, Ni, Cr.
- ❑ Lattice / elastic constants, and SFE in Fe, Ni, Cr.
- ❑ H swelling volume in Fe, Ni, Cr.
- ❑ H diffusion energy barriers in Fe, Ni, Cr.
- ❑ H-vacancy and H-interstitial energies in Fe, N, Cr.
- ❑ H trapping energies in Fe, Ni, Cr.

Zhou et al, J. Comp. Chem., 39, 2420 (2018).



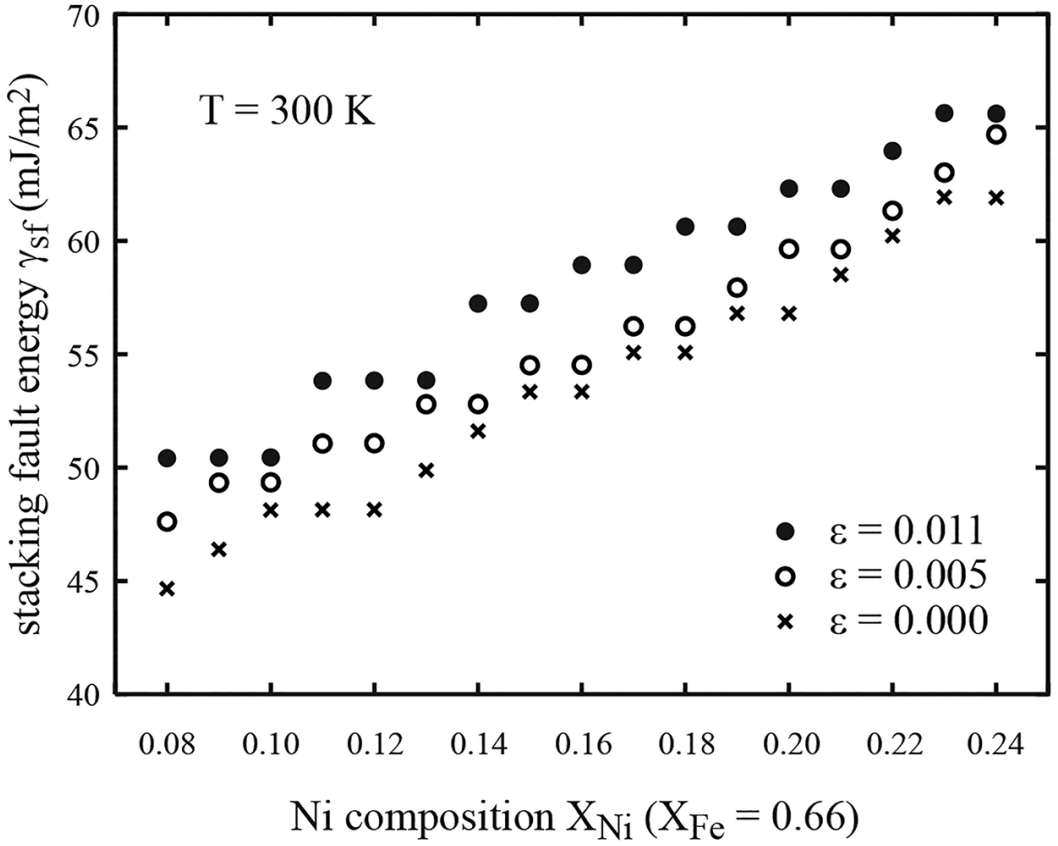
Stability of Structures



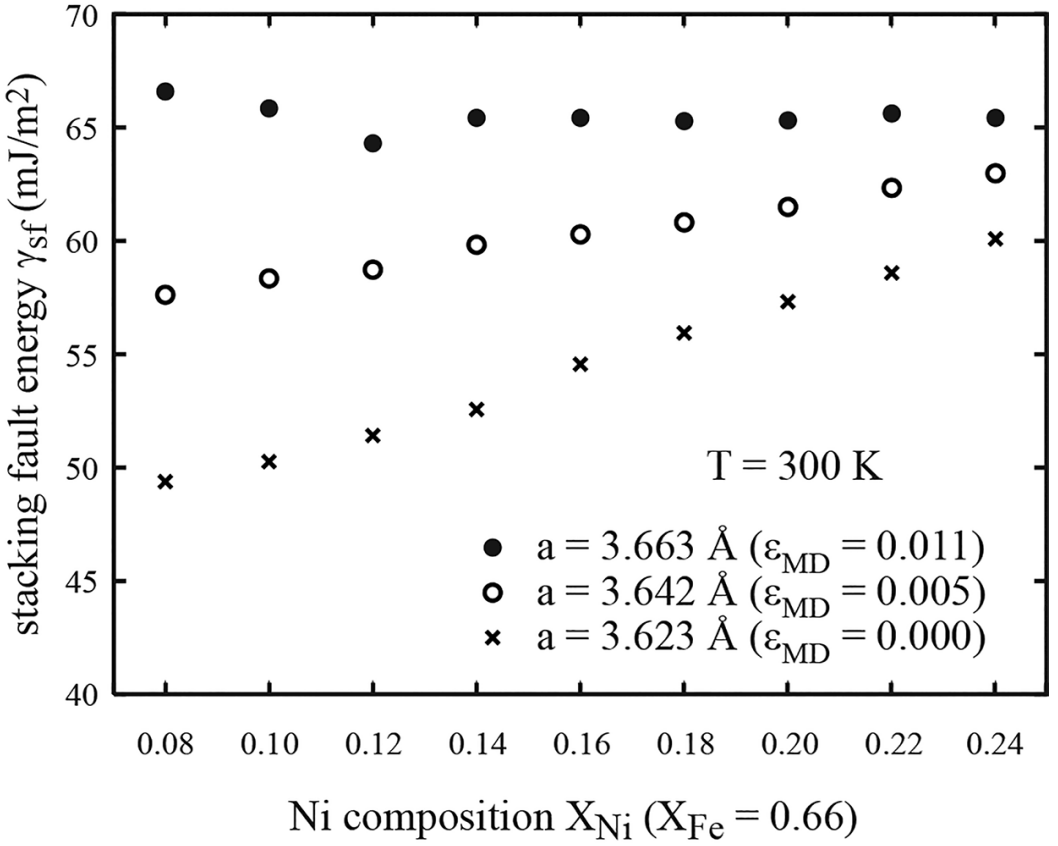
Stability is tested using the most stringent growth simulations.

Stacking Fault Energy

From Potential

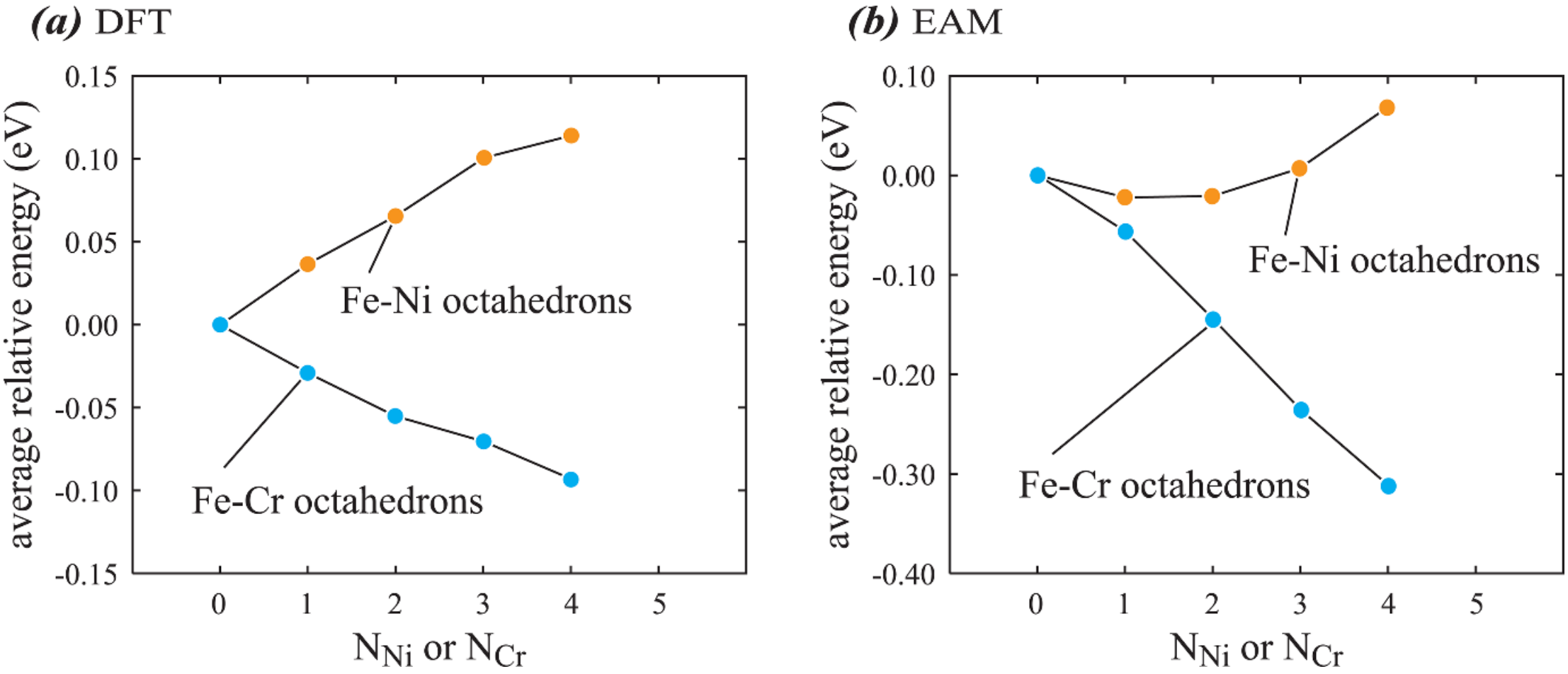


From DFT



Positive slope of SFE with Ni composition is achieved.

H-Metal Interaction Energies

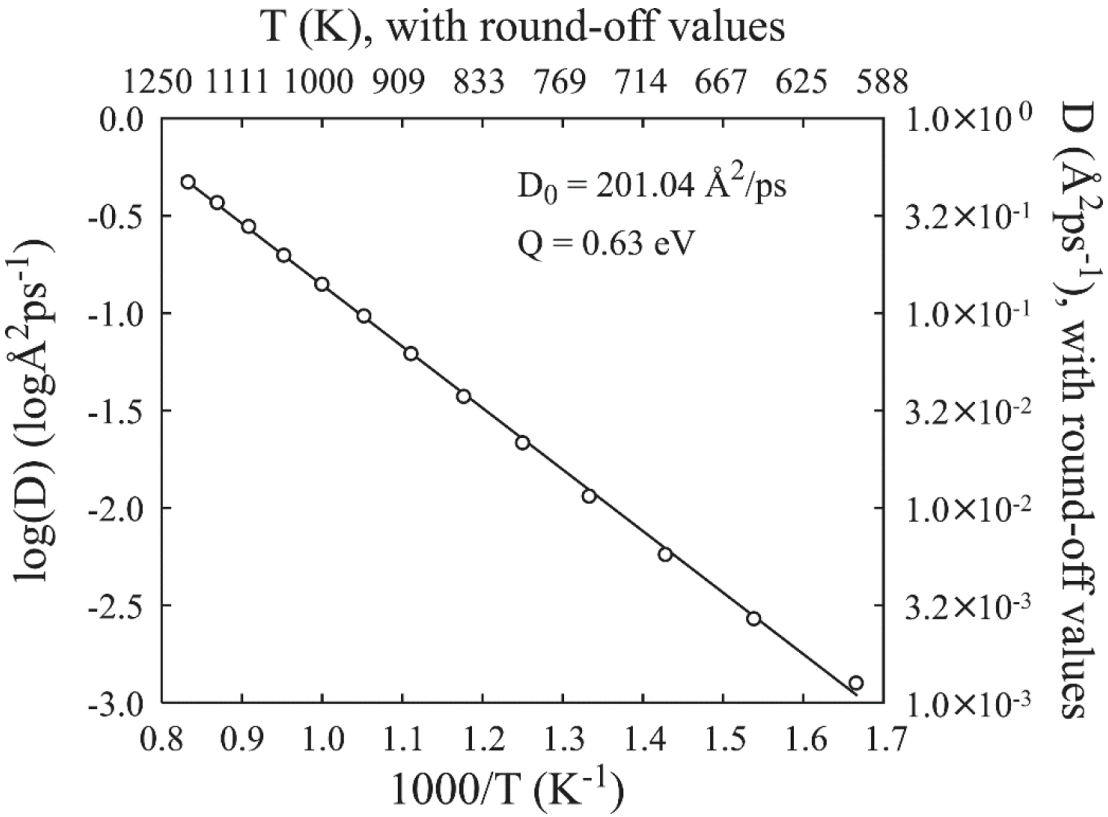


Capture DFT trends that Cr attracts H and Ni repels H.

Statistically-Averaged Diffusivities

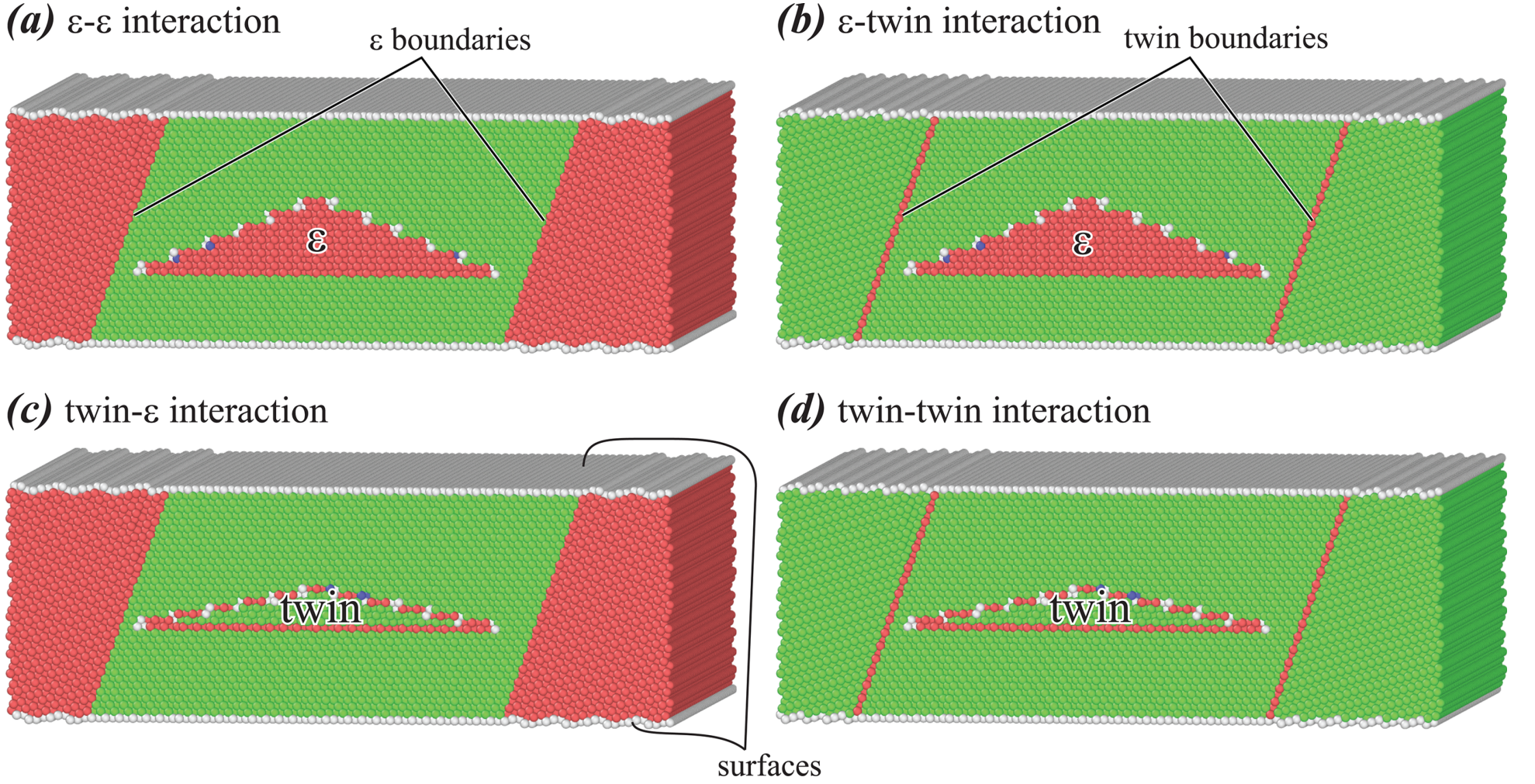
$$\begin{cases} MSD_{1D}(k\Delta t) = \dfrac{\sum_{i=1}^{N}\sum_{j=0}^{m-k}\left[\Delta\alpha_{i,j}^2(k\Delta t)\right]}{N(m+1-k)} \\ MSD_{2D}(k\Delta t) = \dfrac{\sum_{i=1}^{N}\sum_{j=0}^{m-k}\left[\Delta\alpha_{i,j}^2(k\Delta t)+\Delta\beta_{i,j}^2(k\Delta t)\right]}{N(m+1-k)} \\ MSD_{3D}(k\Delta t) = \dfrac{\sum_{i=1}^{N}\sum_{j=0}^{m-k}\left[\Delta x_{i,j}^2(k\Delta t)+\Delta y_{i,j}^2(k\Delta t)+\Delta z_{i,j}^2(k\Delta t)\right]}{N(m+1-k)} \end{cases}$$

$$\begin{cases} D_{1D} = \dfrac{1}{2}\dfrac{dMSD_{1D}(t)}{dt}\Big|_{t\to 0} \\ D_{2D} = \dfrac{1}{4}\dfrac{dMSD_{2D}(t)}{dt}\Big|_{t\to 0} \\ D_{3D} = \dfrac{1}{6}\dfrac{dMSD_{3D}(t)}{dt}\Big|_{t\to 0} \end{cases}$$



- MD accounts for statistics of alloys.
- Calculated barrier 0.63 eV agrees well with the measured 0.51 eV: San Marchi et al, Inter. J. Hydro. Ener., 32, 100 (2007).

Experimental Validation: Slip Band Collision Simulations



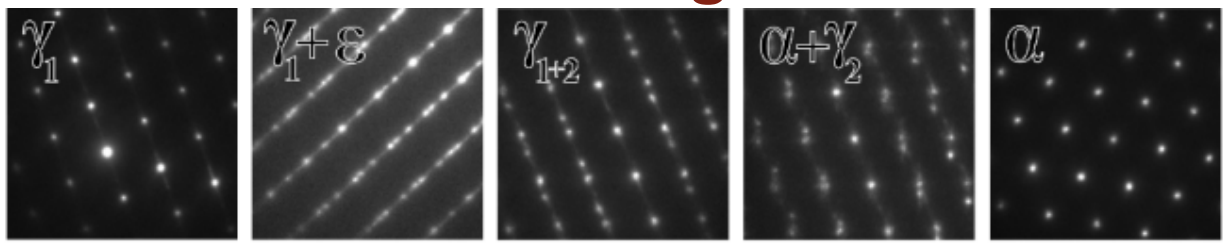
Experimentally, the material deforms through formation and extension of slip bands.

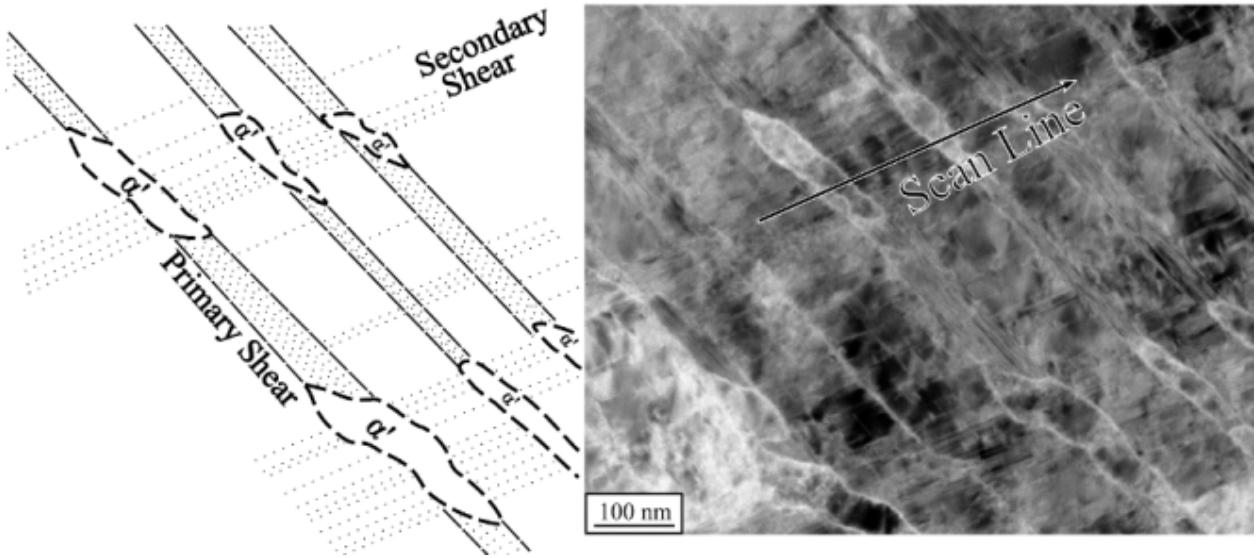
Simulations of slip band collision provide a good problem to validate our potential.

Slip band collision occurs when a shear stress is applied to the surfaces in our MD model.

Validation: α’ Martensite Formation

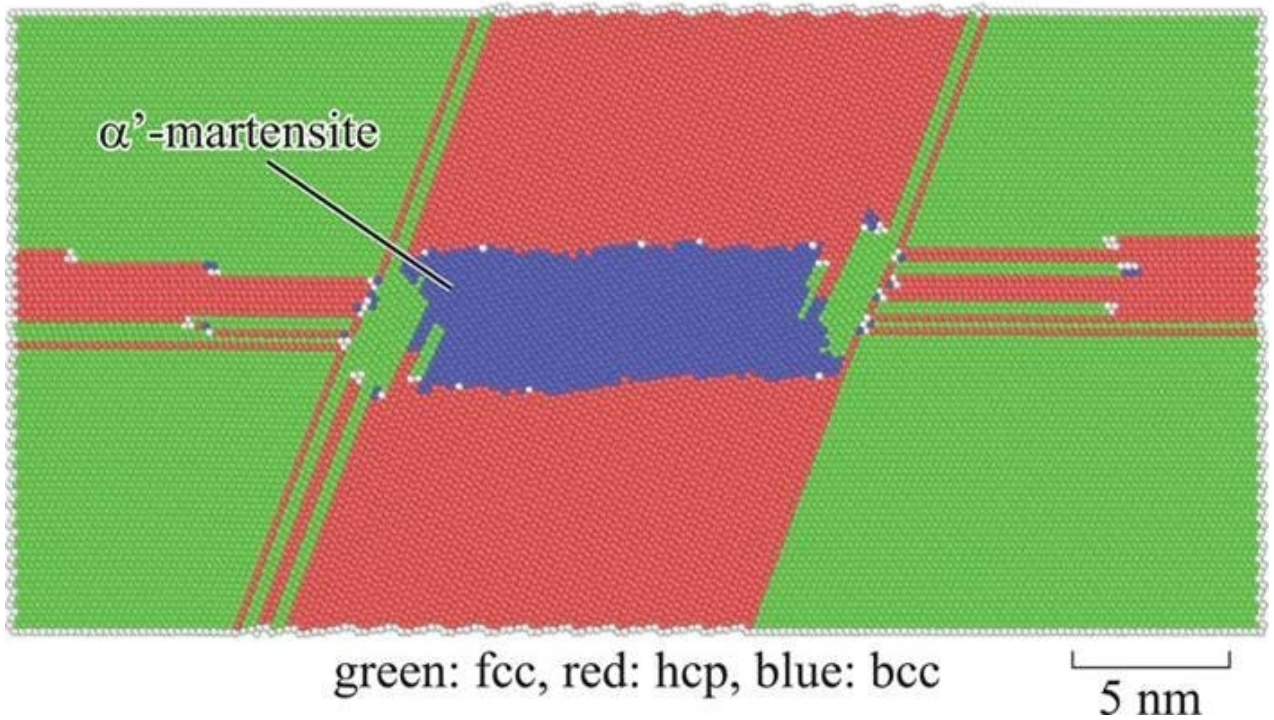
Transmission electron microscope (TEM) from Doug Medlin





Molecular dynamics (MD)

collision of an ε-martensite band (screw Burgers vector) with an ε-martensite band at τ = 1.15 GPa



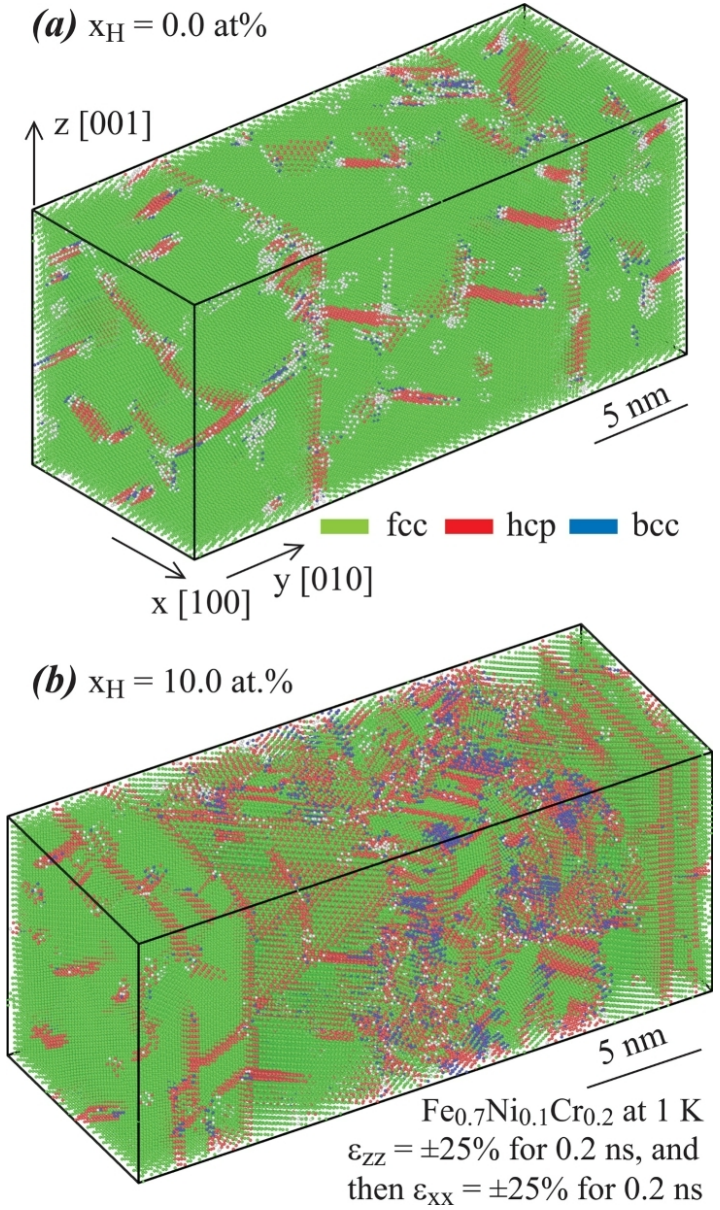
Both TEM and MD show:

$$\{111\}_\gamma // \{0001\}_\epsilon // \{011\}_{\alpha'}$$

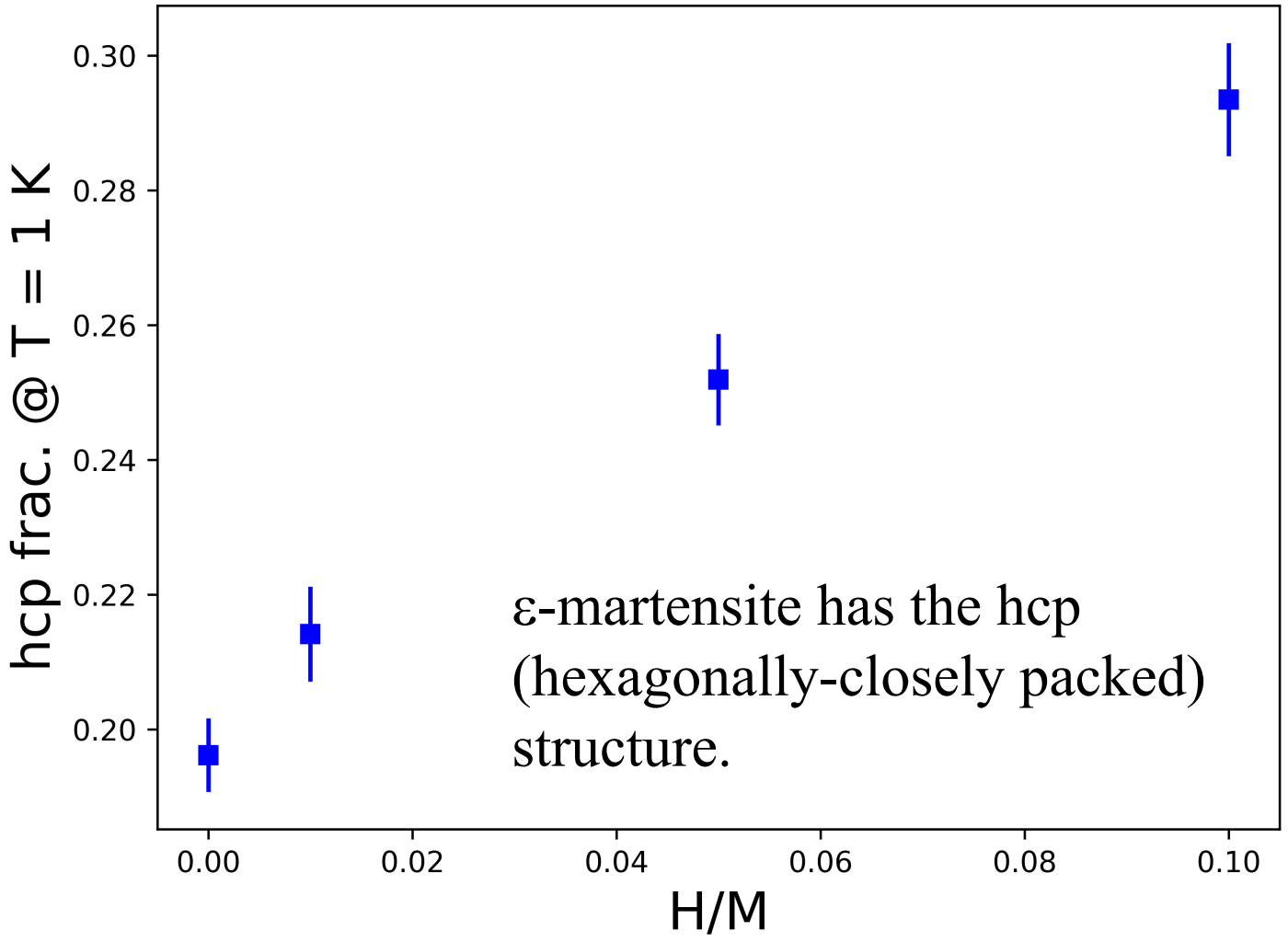
$$\langle 110\rangle_\gamma // \langle 11\bar{2}0\rangle_\epsilon // \langle 111\rangle_{\alpha'}$$

Validation: H promotes ε-Martensite Slip Band

MD configurations

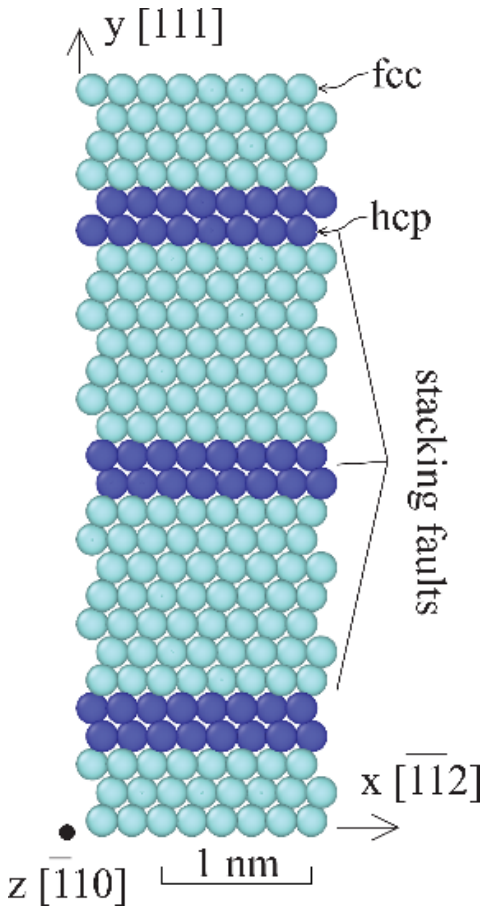


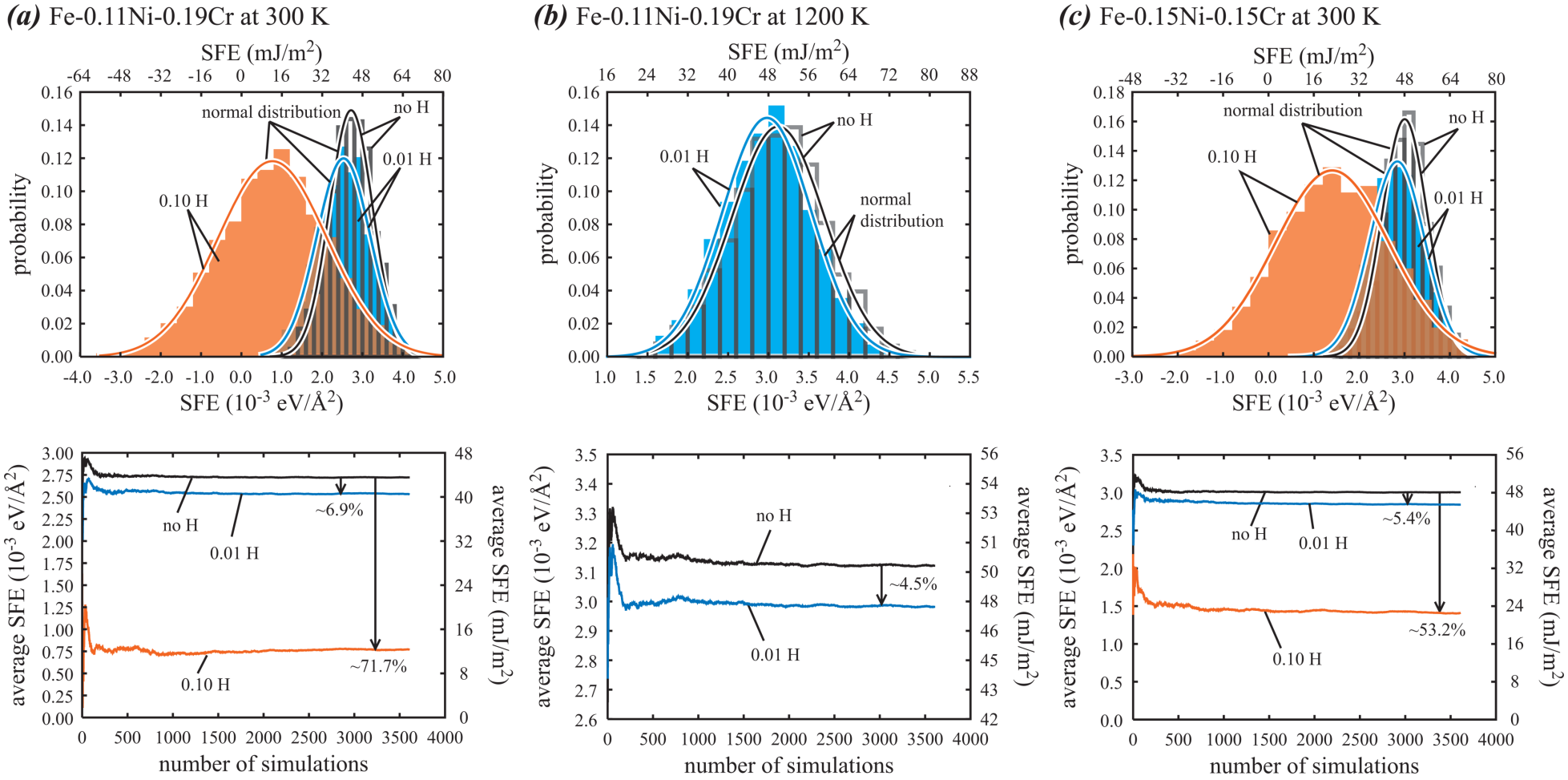
MD predicted ε-martensite fraction vs. H content



Experiments indicate that H promotes ε-martensite slip bands, Metall. Mater. Trans. A, 52, 1516 (2021).

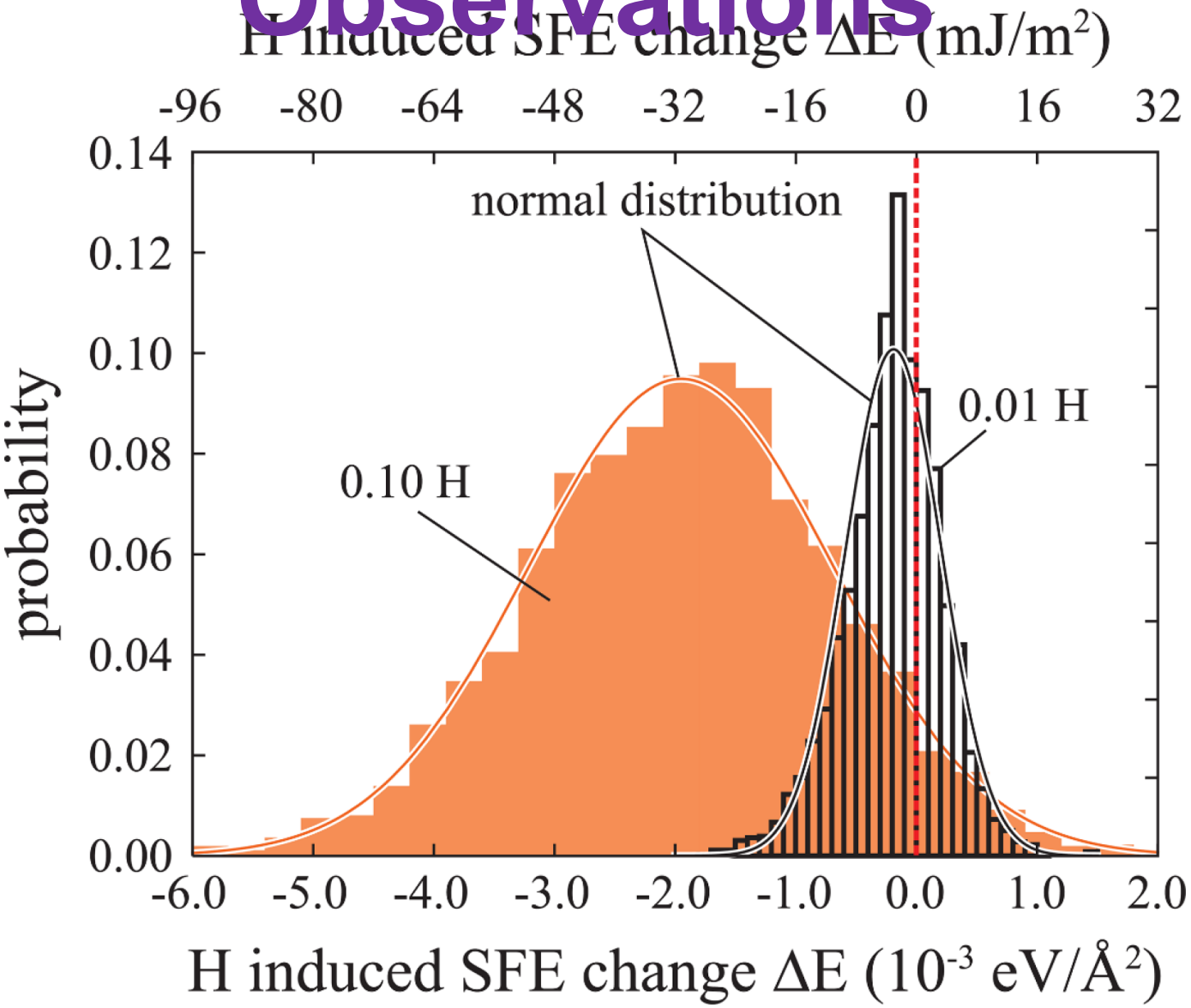
SFE Distributions from 57600 MD Simulations



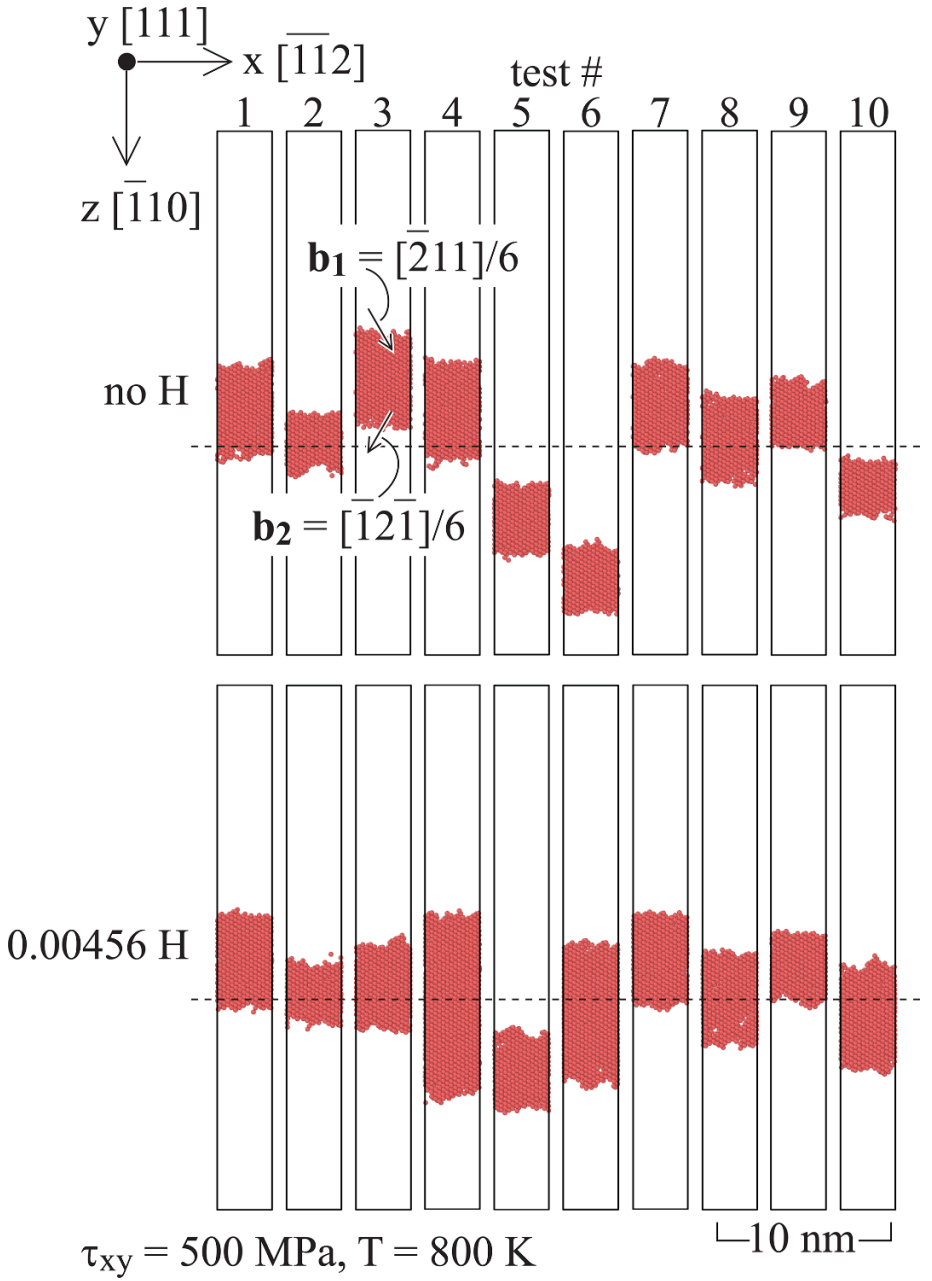


Stacking fault energy based alloy screening for hydrogen compatibility: Gibbs et al,. JOM, 72, 1982 (2020).

Additional Observations



After 1.8 ns MD simulations

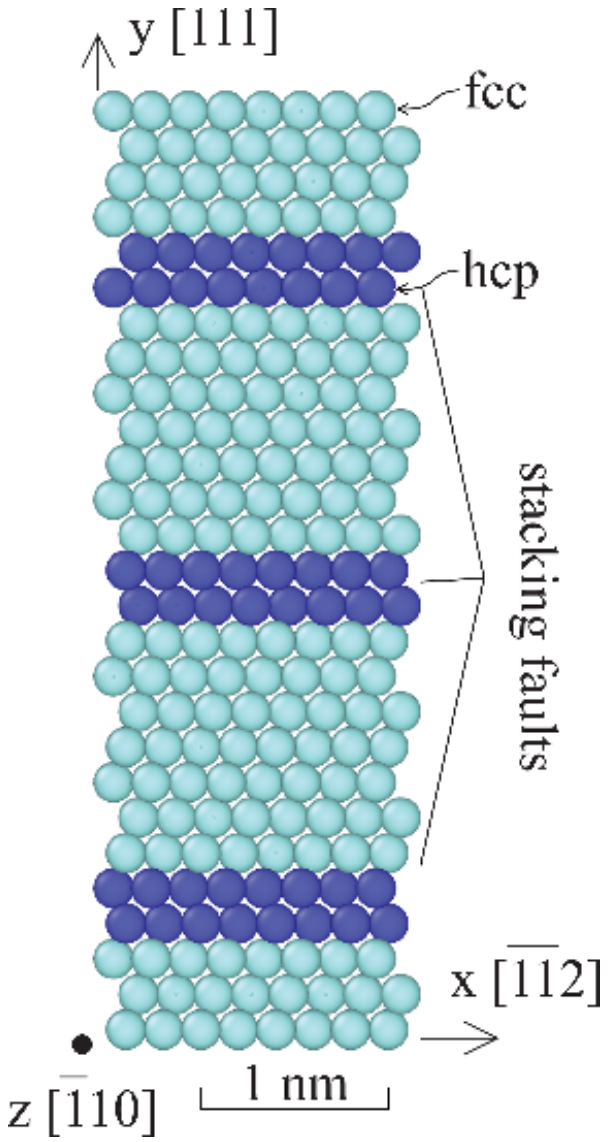


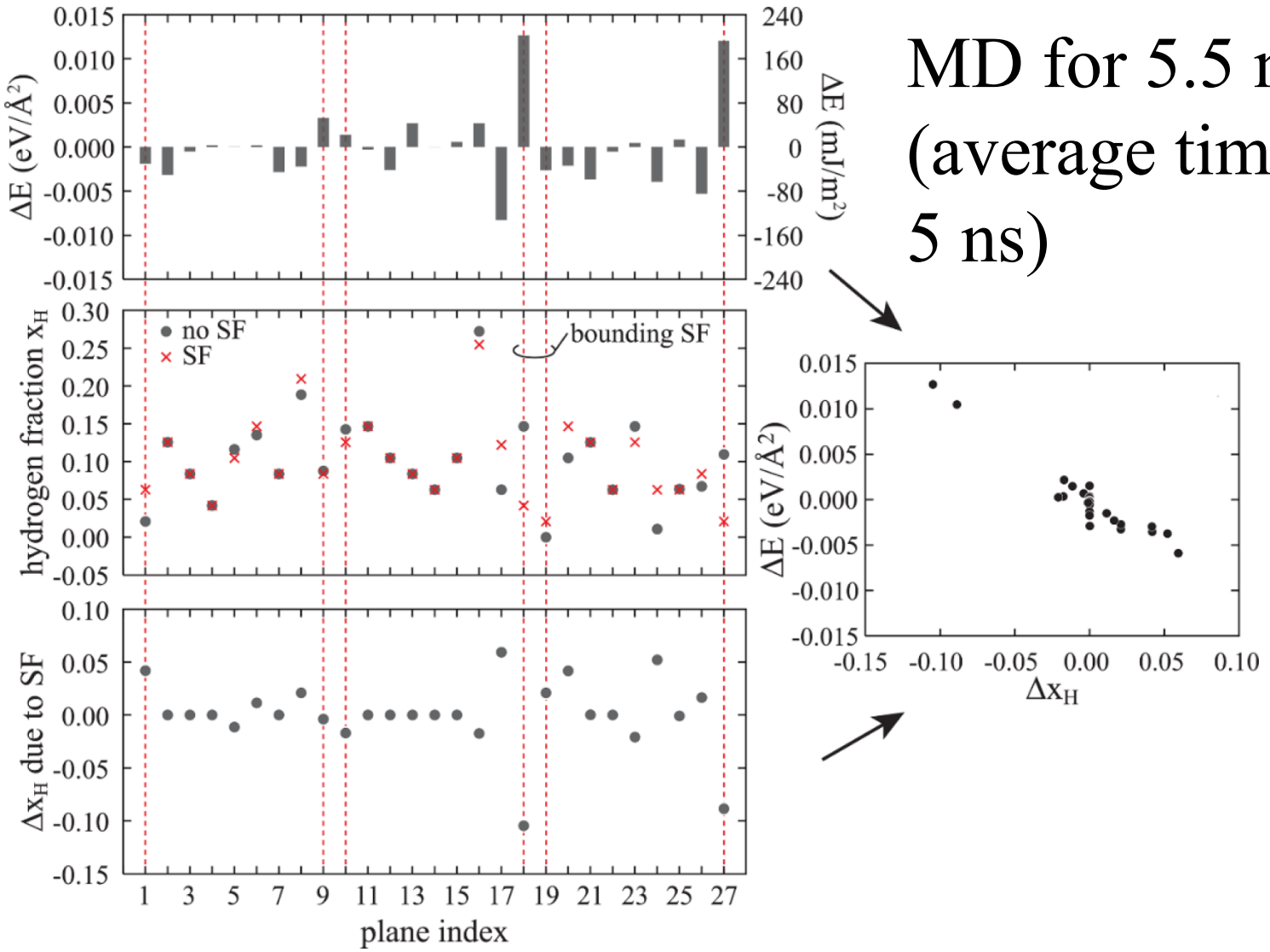
SUMMARY

1. An Fe-Ni-Cr-H potential suitable for studying SFE and the related slip bands has been developed.
2. This potential reproduces the experimentally observed H effects on ε- and α'- martensite formation in slip bands.
3. SFE in stainless steels is not a single value, but rather is a distribution due to local composition variations.
4. Hydrogen significantly reduces the mean SFE, in agreement with experiments.
5. Previous views on SFE effects are too simplistic.

Spare Slides

Plane-Resolved Energies

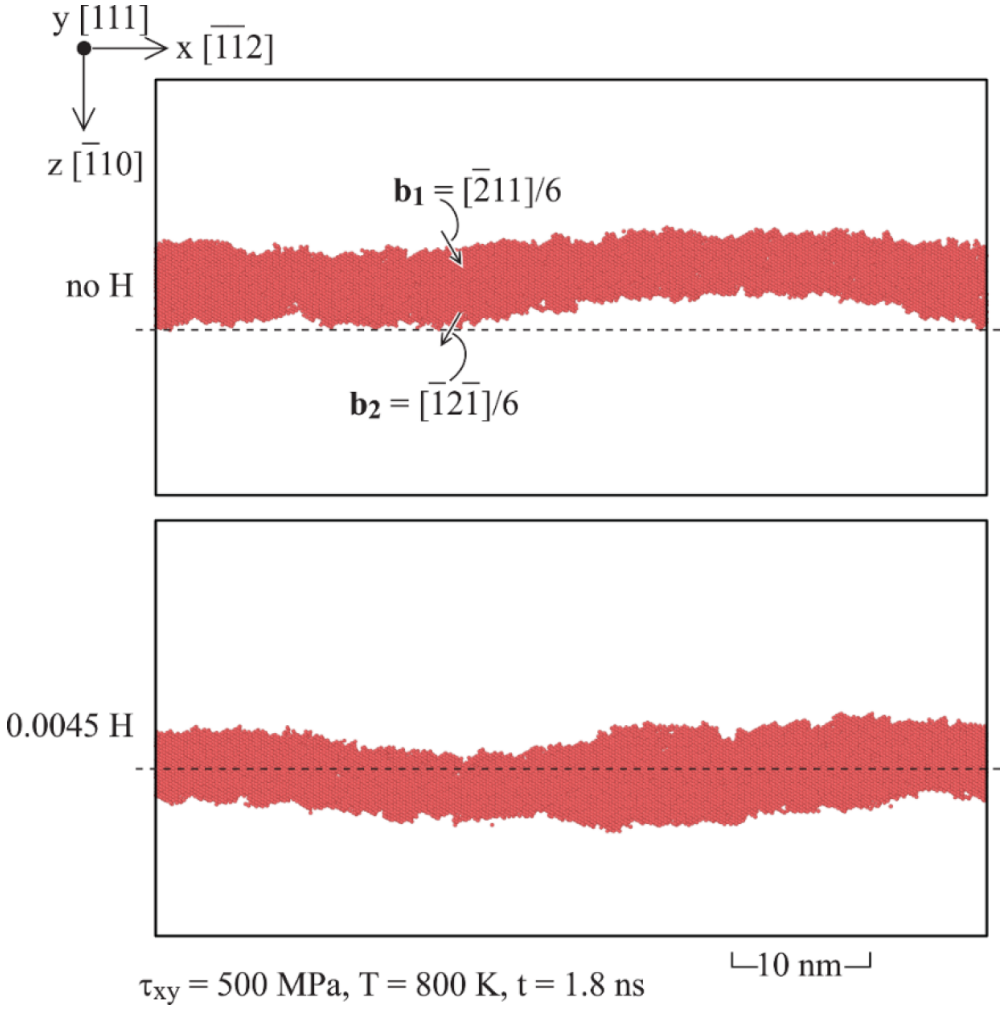




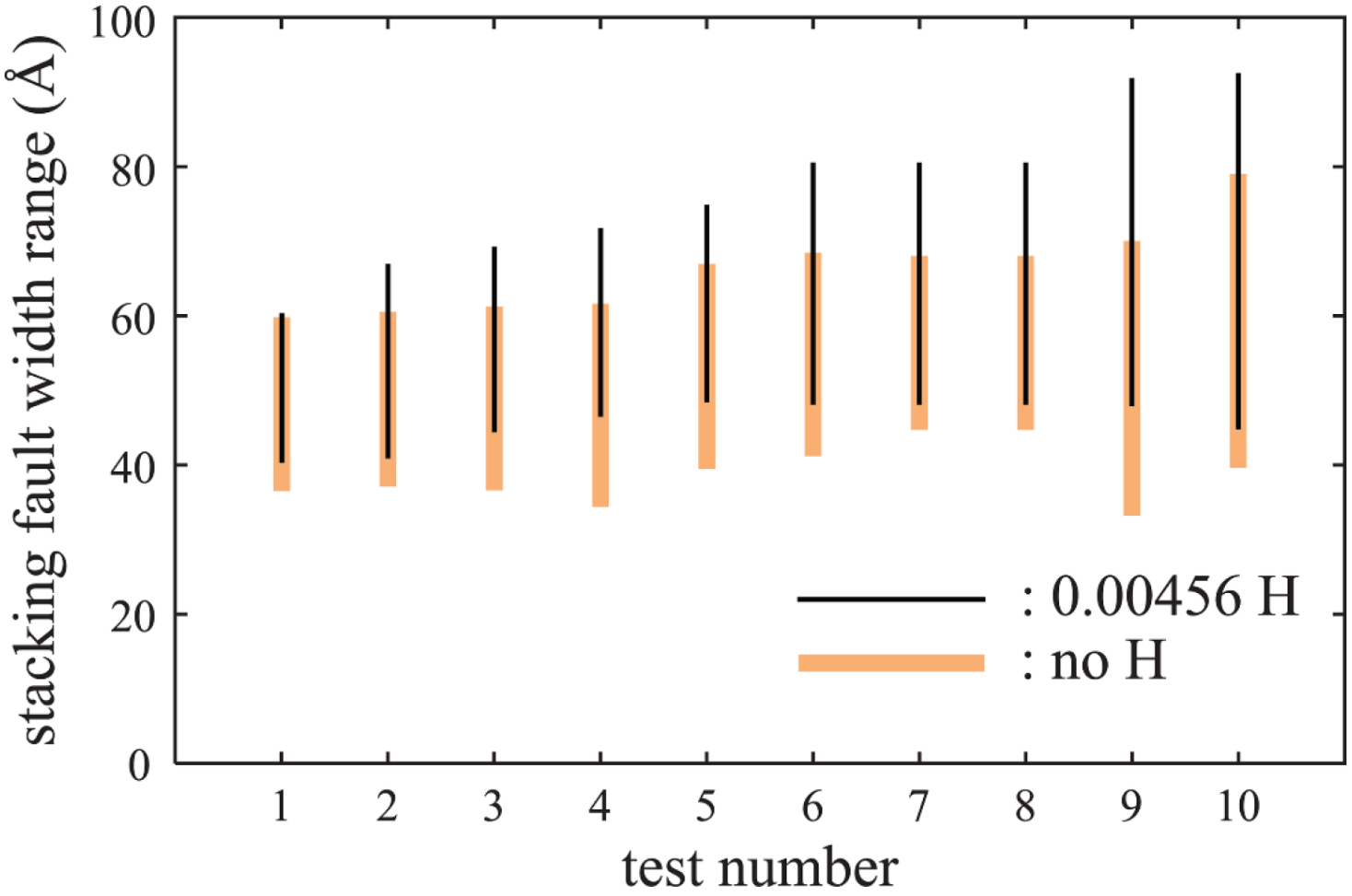
MD for 5.5 ns (average time 5 ns)

Stacking Fault Width of Long Dislocations

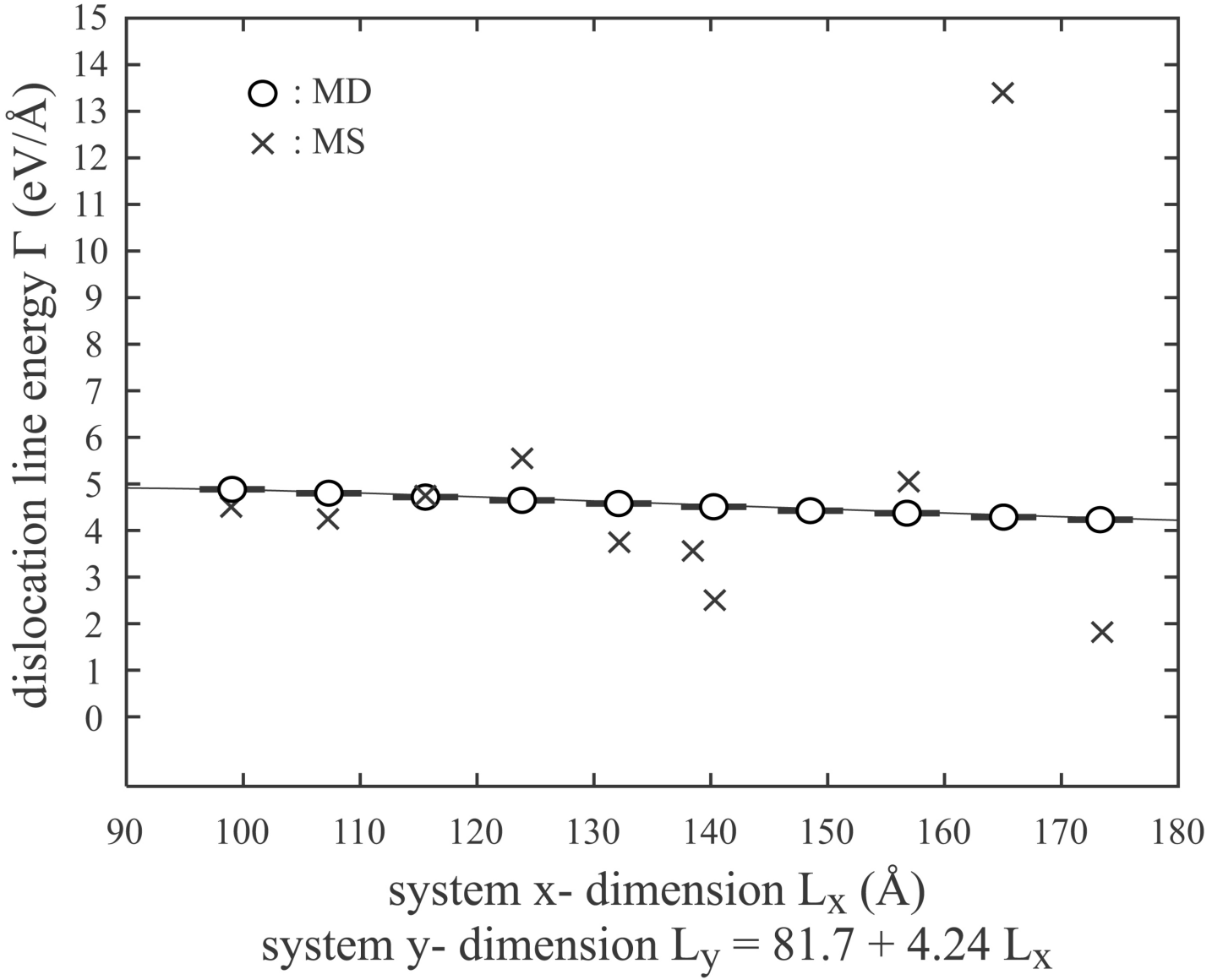
H effects on MD configurations



Stacking fault width range from 10 replicas



Errors of (Time-Averaged) MD vs. MS



1. X. W. Zhou, and M. E. Foster, Phys. Chem. Chem. Phys., 2021, 23, 3290.

2. X. W. Zhou, D. K. Ward, J. A. Zimmerman, J. L. Cruz-Campa, D. Zubia, J. E. Martin, and F. van Swol, J. Mech. Phys. Solids, 2016, 91, 265.