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Towards Machine-Learning of Hydrogen Effects on Stacking Fault Energies in Austenitic Stainless Steels

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Stacking Fault Energy (SFE) on Hydrogen Embrittlement

- SFE is related to hydrogen compatibility parameter RRA (relative reduction in area)[1].
  - RRA > 80% when SFE > 40 mJ/m^2;
  - RRA ~ 20-80% when SFE ~ 20-40 mJ/m^2.
- The austenitic stainless steels deform through hydrogen-mediated slip bands[2].
- Experimentally, hydrogen reduces SFE. Density functional theory (DFT) calculations on small scales do not clearly show this.
- DFT does not address effects such as hydrogen "cloud" characteristics, alloy local composition distribution, repopulation of hydrogen upon stacking fault formation, hydrogen segregation, temperature, and others ....

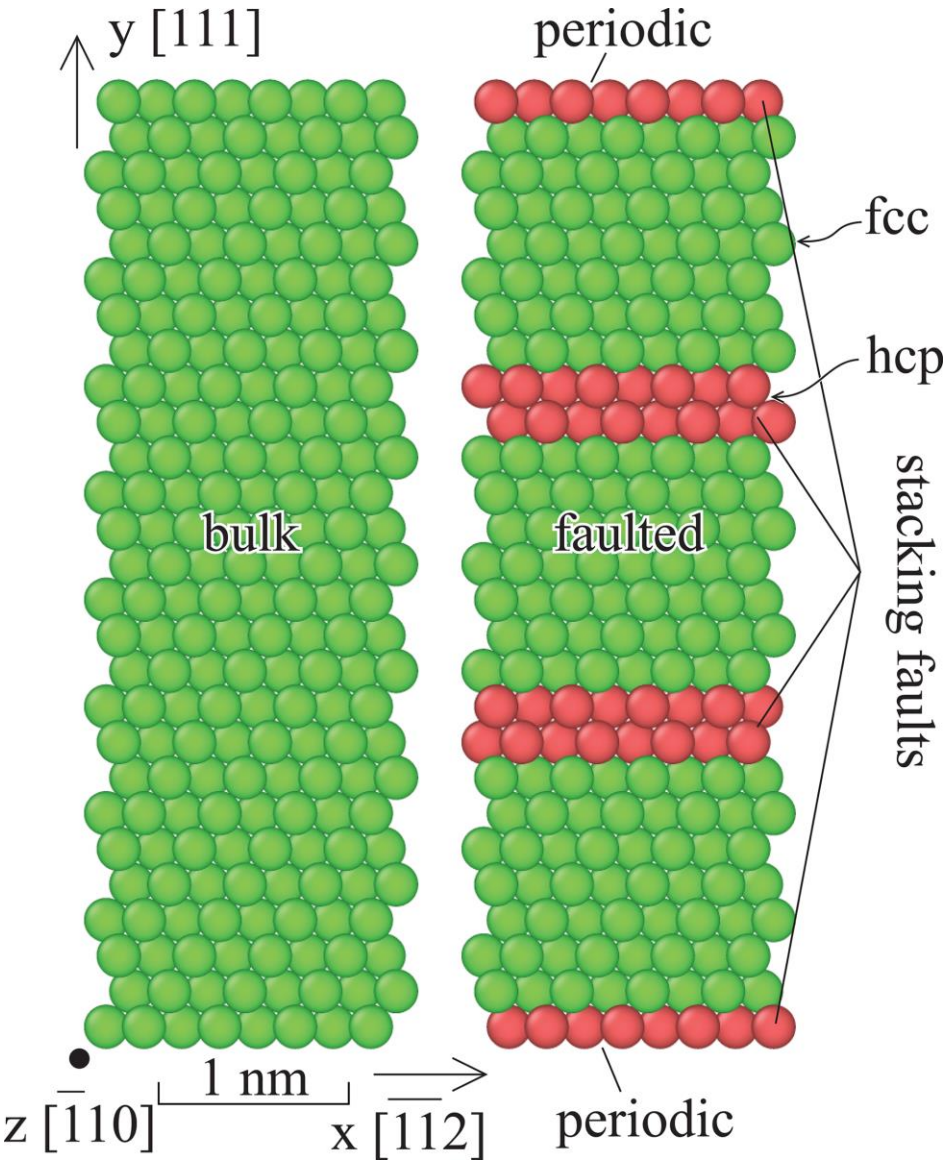
[1] Gibbs et al, JOM, 72, 1982 (2020), [2] Sabisch et al, Metall. Mater. Trans. A, 52, 1516 (2021).

Molecular Dynamics (MD) Advantages / Readiness

- Large, ensemble simulations capture local alloy composition distributions.
- Time – averaged MD (rather than energy minimization) simulations capture hydrogen "cloud" effects.
- Time-averaged MD is far more accurate than energy minimization[1,2].
- Enable hydrogen repopulation upon stacking fault formation, and non-uniform segregation of hydrogen.
- Literature Fe-Ni-Cr-H potential[3] has captured (a) lattice / elastic constants, and SFE in Fe, Ni, Cr, and (b) hydrogen relative energies, swelling volumes, diffusion energy barriers, and H-point defect energies in Fe, Ni, Cr.

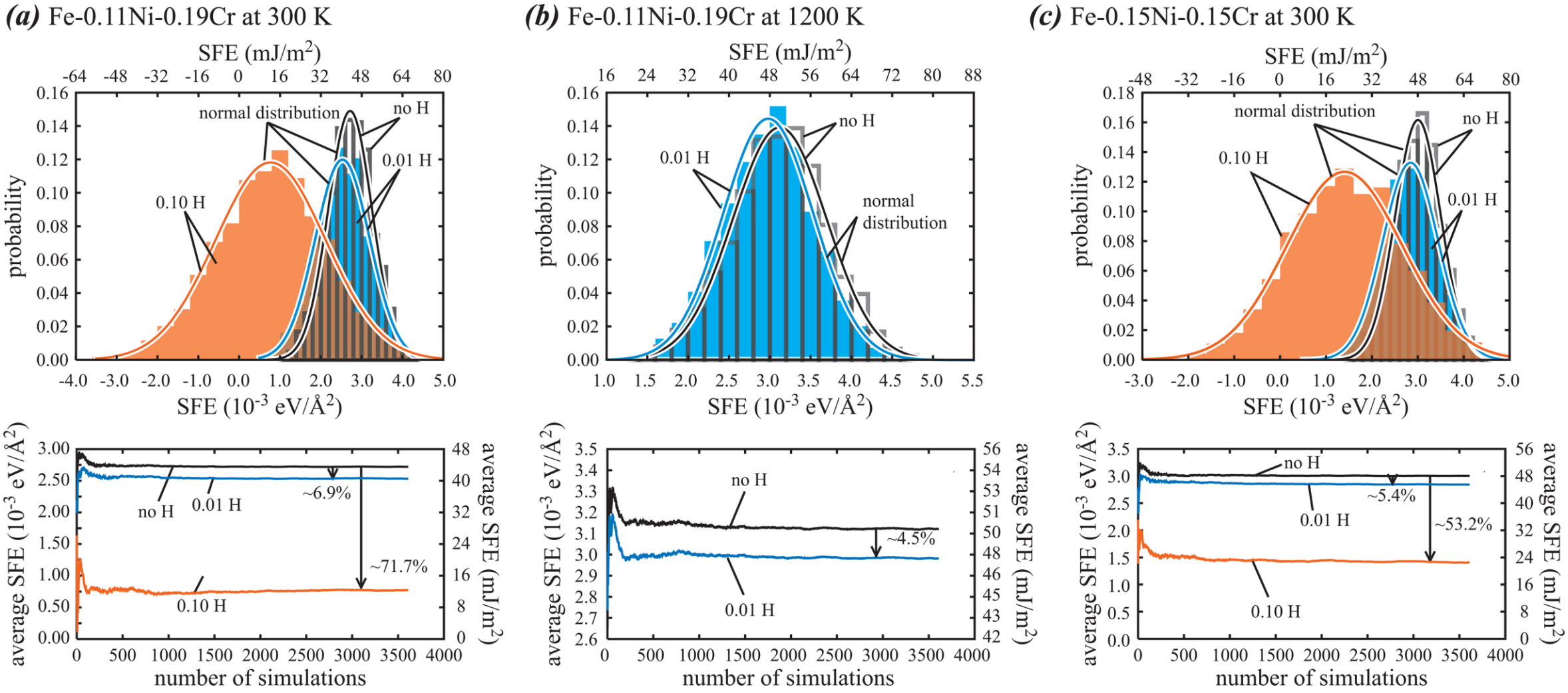
[1] Zhou el al, Phys. Chem. Chem. Phys., 23, 3290 (2021), [2] Zhou et al, J. Comp. Chem., 39, 2420 (2018), [3] Zhou et al, J. Mech. Phys. Solids, 91, 265 (2016).

MD Simulation Methodology



- Small x-z dimension is used to sample local alloy composition given an overall composition.
- Three stacking faults (SF) are used so correlated bulk and faulted systems can be created.
- Energies are overaged over 5 ns using time-averaged MD simulations.
- SFE is calculated as the energy difference between bulk and faulted systems per unit of stacking fault area.
- 3600 SFE values obtained from different random number seeds are used to study distribution.

SFE Results

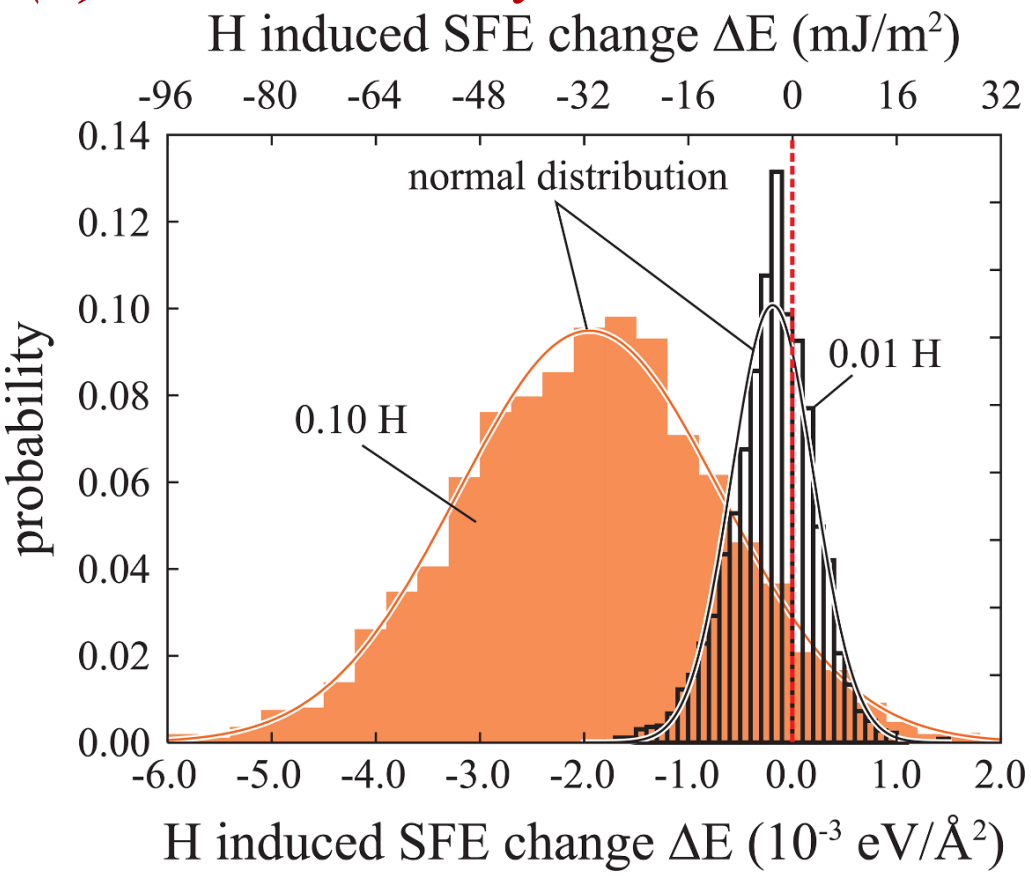


- SFE in alloys is a distribution in alloys.
- Increasing Ni and temperature increases SFE.
- Hydrogen reduces mean SFE.
- These agree with experiments[1-5].

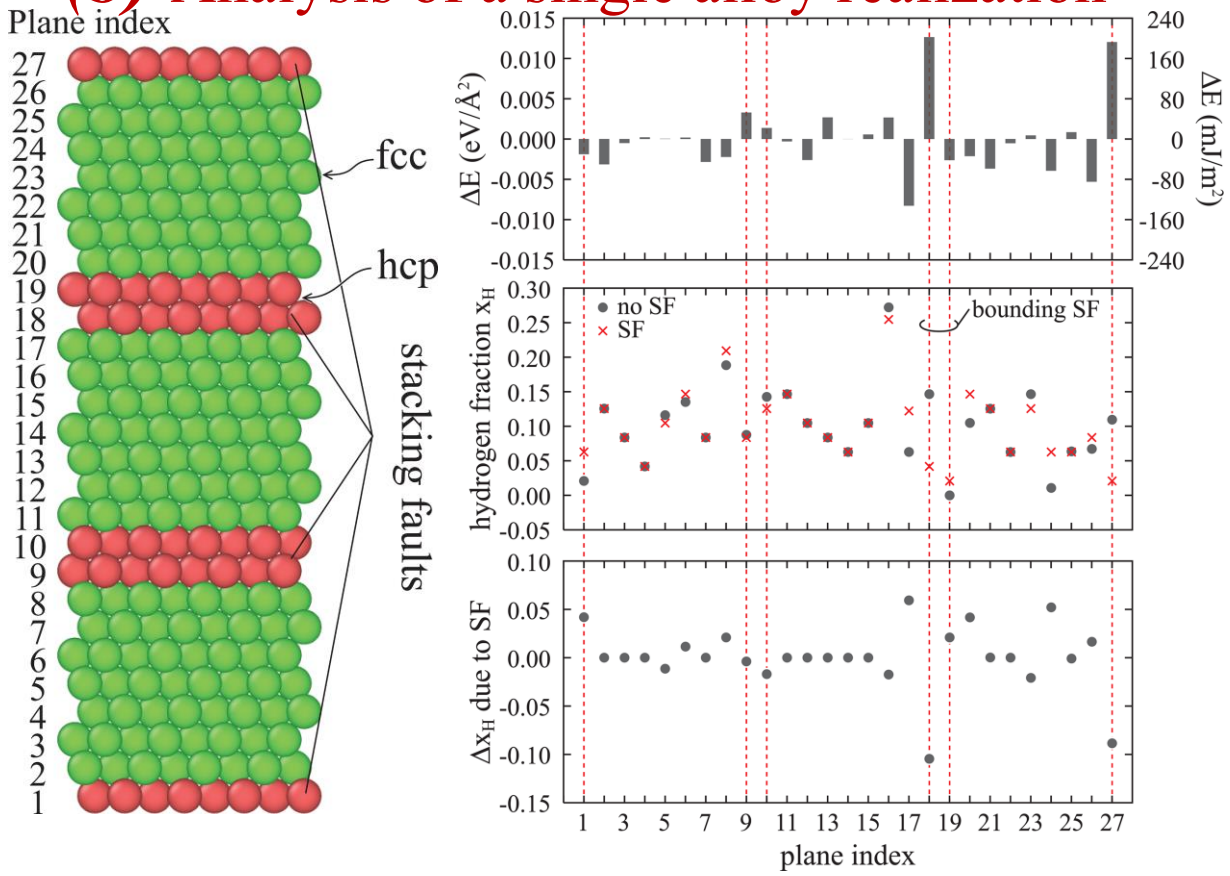
[1] Vitos et al, Phys. Rev. Lett. 96, 117210 (2006), [2] Latanision et al, Metall. Trans., 2, 505 (1971). [3] Molnar et al, Mater. Sci. Eng. A., 759, 490 (2019). [4] Barannikova et al, Tech. Phys. Lett., 37, 793 (2011). [5] Kuprekova et al, Metal Sci. Heat Treat., 50, 282 (2008).

Hydrogen (H) Effects

(a) from 3600 alloy realizations



(b) Analysis of a single alloy realization



- H can increase or decrease local SFE, but reduces average SFE from many alloy realizations.
- For a given realization, H changes the SFE through a plane-by-plane contributions.
- The plane-by-plane contribution can be ±, with the largest magnitude occurs near SF.
- H repopulates upon SF formation. Largest change of H concentration occurs near SF.

Our Database for Hydrogen Effects

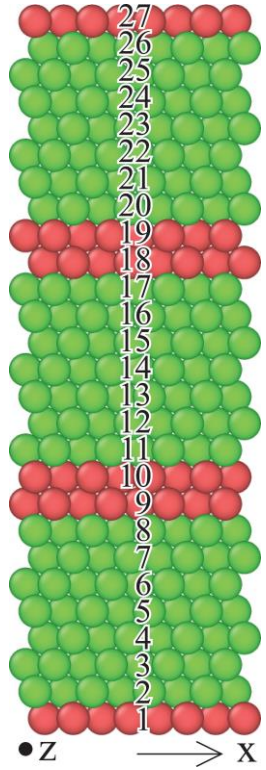
One of 3600 tables is listed, where highlighted planes bounds SF.

SFE = 2.497 meV/Å^2, X_{Fe} = 0.7029, X_{Ni} = 0.1065, X_{Cr} = 0.1906, X_H = 0.0093, L_x = 17.7848 Å, L_z = 15.3839 Å

Plane #	X_H without SF	X_H with SF	N_a without SF	E_a without SF (eV)	N_a with SF	E_a with SF (eV)
1	0.0000	0.0105	48.0000	-4.3582	48.5038	-4.3391
2	0.0004	0.0004	48.0198	-4.3342	48.0195	-4.3283
3	0.0216	0.0212	49.0388	-4.2912	49.0180	-4.2919
4	0.0199	0.0201	48.9534	-4.2971	48.9626	-4.2940
5	0.0206	0.0040	48.9880	-4.2790	48.1941	-4.3176
6	0.0000	0.0168	48.0000	-4.3419	48.8059	-4.3095
7	0.0000	0.0000	48.0000	-4.3007	48.0000	-4.3014
8	0.0000	0.0000	48.0000	-4.3354	48.0000	-4.3313
9	0.0000	0.0000	48.0000	-4.3245	48.0000	-4.3222
10	0.0009	0.0059	48.0412	-4.3350	48.2844	-4.3231
11	0.0172	0.0149	48.8259	-4.3317	48.7156	-4.3320
12	0.0028	0.0000	48.1329	-4.3179	48.0000	-4.3241
13	0.0030	0.0027	48.1447	-4.3583	48.1311	-4.3591
14	0.0222	0.0225	49.0671	-4.2805	49.0796	-4.2788
15	0.0164	0.0164	48.7881	-4.2899	48.7894	-4.2901
16	0.0000	0.0000	48.0000	-4.3563	48.0000	-4.3560
17	0.0023	0.0013	48.1103	-4.3246	48.0625	-4.3233
18	0.0185	0.0195	48.8897	-4.3009	48.9375	-4.2928
19	0.0032	0.0109	48.1529	-4.3704	48.5246	-4.3563
20	0.0200	0.0117	48.9603	-4.2623	48.5625	-4.2791
21	0.0210	0.0208	49.0062	-4.3037	48.9982	-4.3046
22	0.0183	0.0191	48.8806	-4.2895	48.9147	-4.2882
23	0.0000	0.0000	48.0000	-4.3359	48.0000	-4.3354
24	0.0009	0.0000	48.0432	-4.3491	48.0000	-4.3445
25	0.0148	0.0030	48.7114	-4.3349	48.1417	-4.3651
26	0.0057	0.0179	48.2717	-4.3209	48.8583	-4.2894
27	0.0203	0.0103	48.9737	-4.3086	48.4962	-4.3143

number of metal atoms per plane = 48

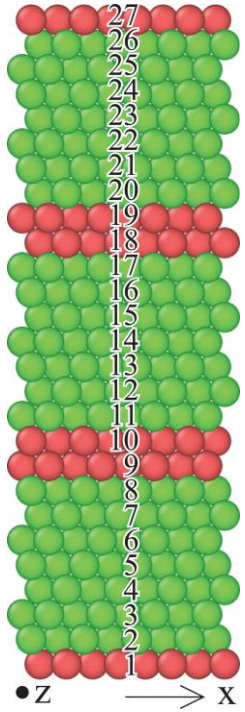
- SFE: stacking fault energy;
- X_{Fe}, X_{Ni}, X_{Cr}, X_H (outside the table) atomic fraction (with respect to total metal atoms);
- L_x, L_z: x and z dimension. Stacking fault area $A = 3L_xL_z$.
- X_H (inside the table): time-averaged atomic fraction on the plane.
- N_a: total number of atoms on the plane.
- E_a: energy per atom on the plane.

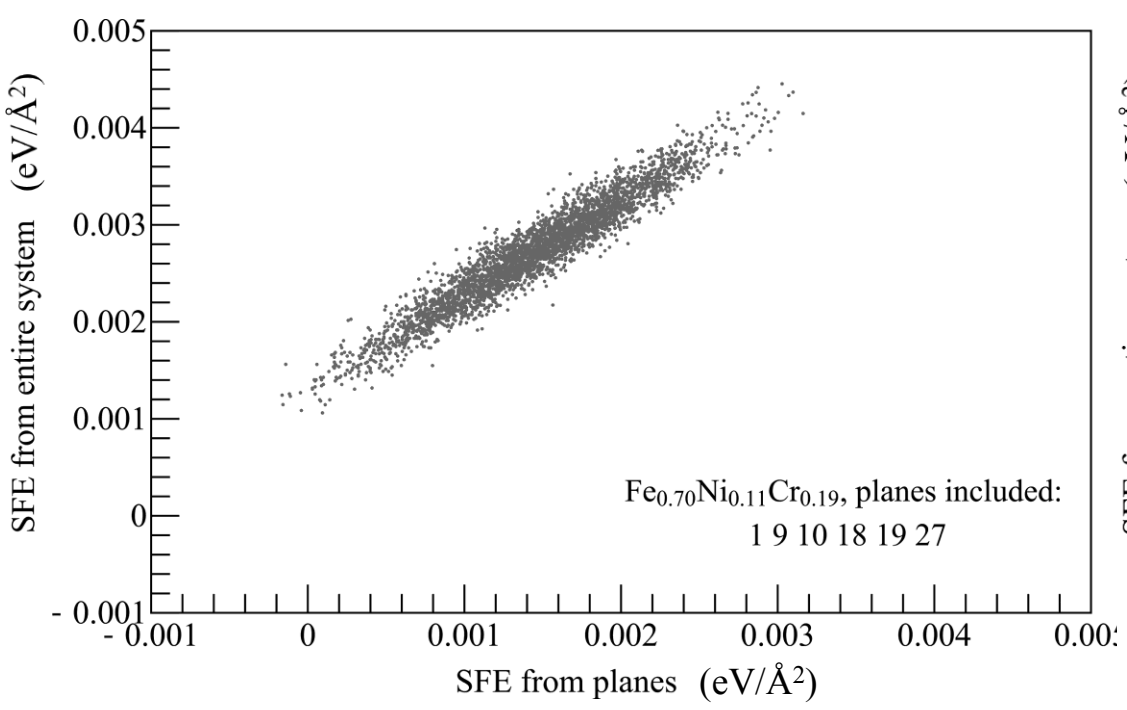


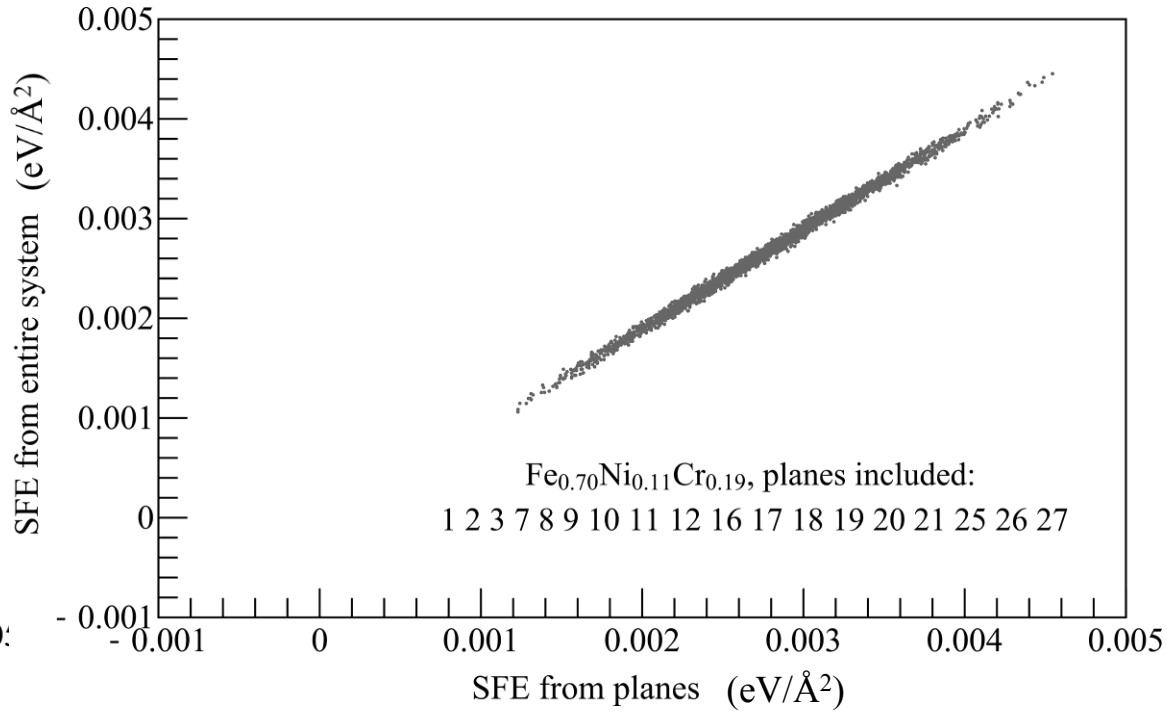
- For each case (given alloy composition and temperature), there are 3600 tables like this from 3600 realizations.
- Question 1: Given local alloy compositions, can ML tell H population with and without SF?
- Question 2: Once H population can be predicted, can ML tell SFE?

SF Range Effects on SFE: $Fe_{0.70}Ni_{0.11}Cr_{0.19}$

Correlation between system SFE and plane contributions



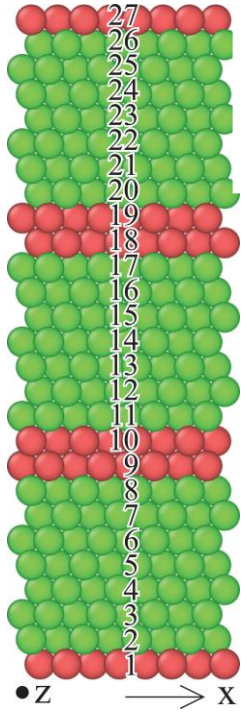


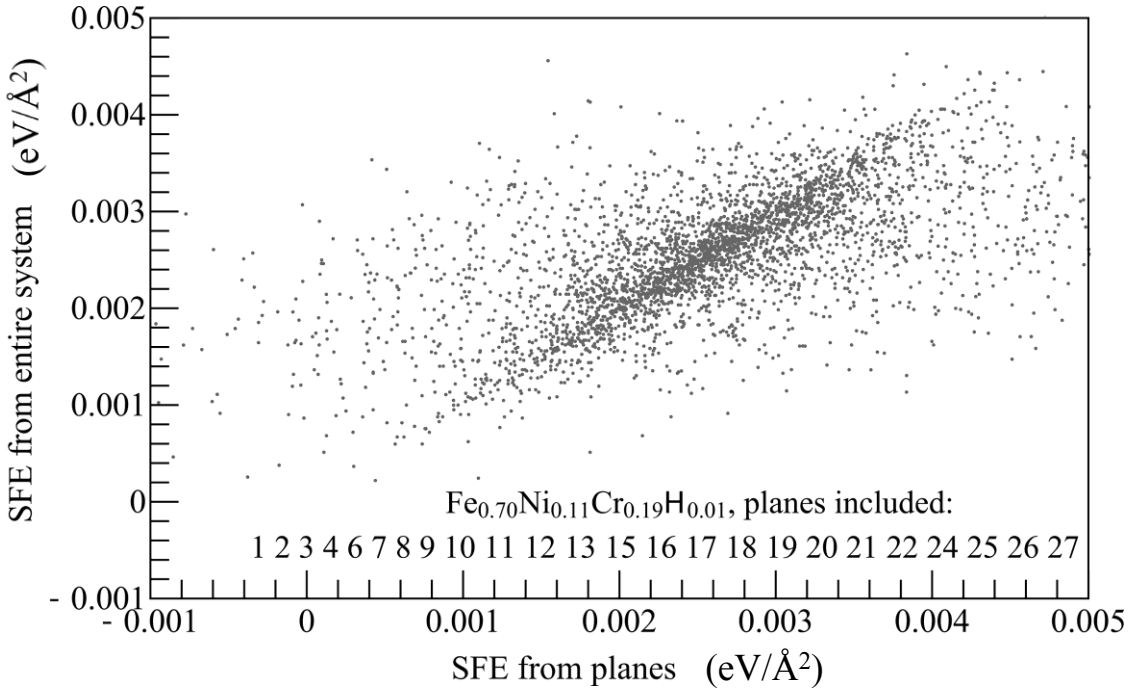


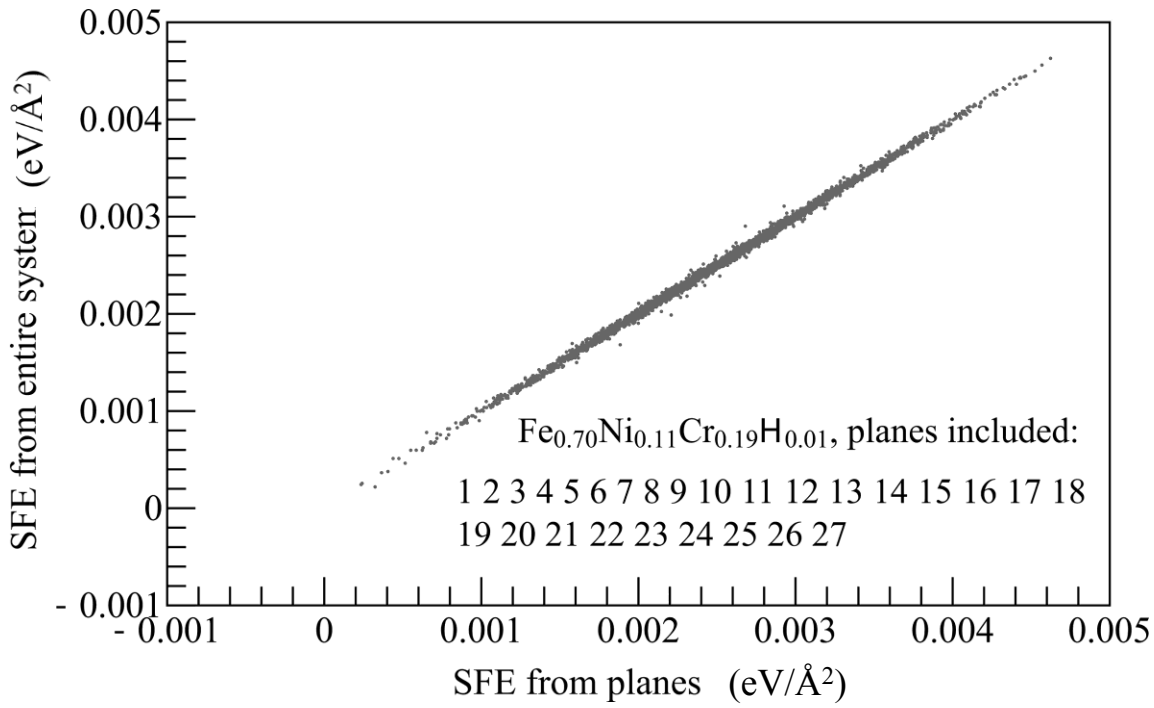
- The total system energy is a summation of energies on all planes.
- Energies on planes are altered by the formation of the three stacking faults.
- SFE can be calculated from total energy change, or energy changes from planes closest to SF.
- From the 3600 H-free systems, SFEs from two planes near the SF already correlate very well with the system SFEs. SFEs calculated from six planes near the SF approach well the system SFEs.

SF Range Effects on SFE: $Fe_{0.70}Ni_{0.11}Cr_{0.19}H_{0.01}$

Correlation between system SFE and plane contributions





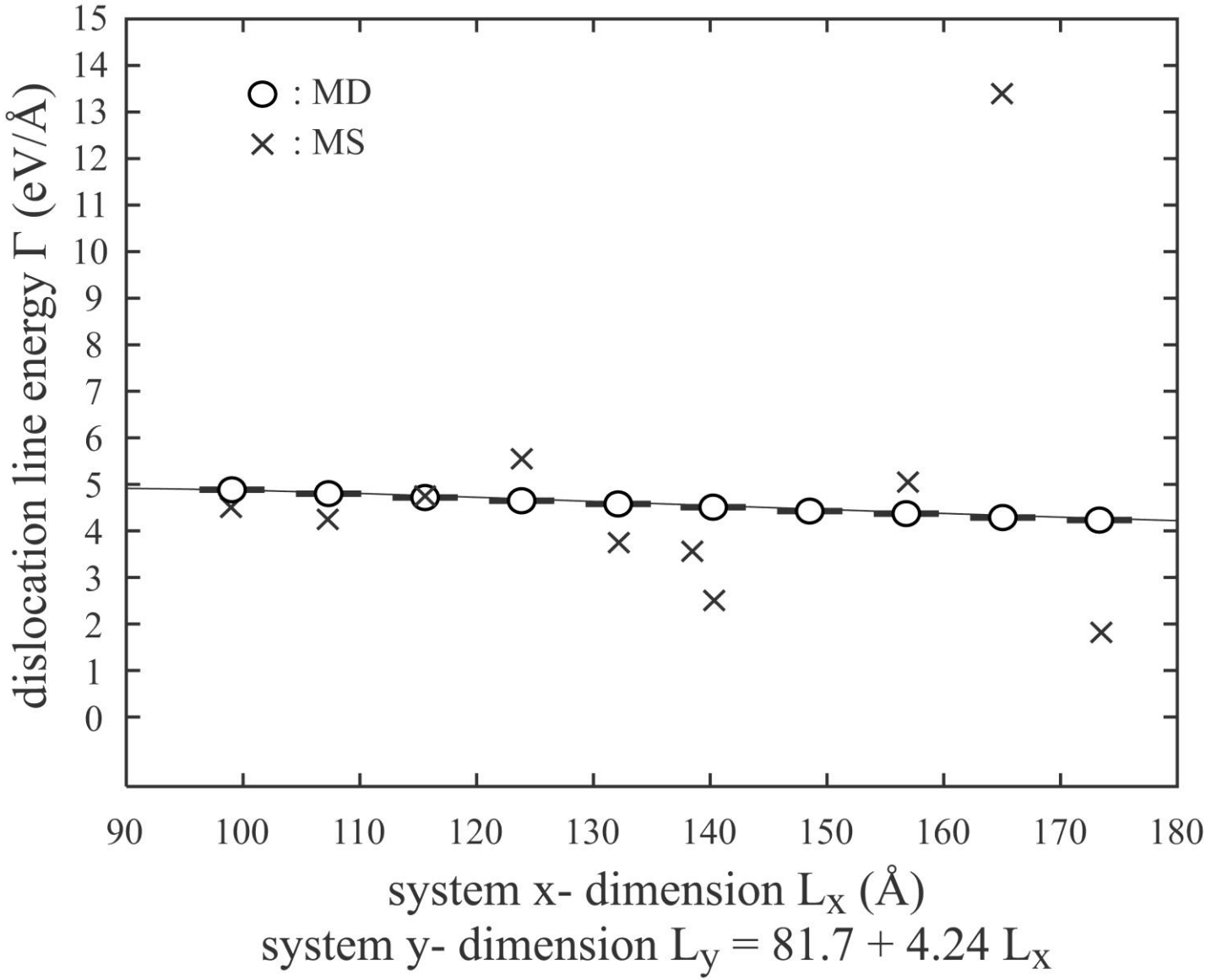


- From the 3600 H-containing systems, the correlation between system and plane SFEs is not well defined even when eight planes near the SF are included.
- SFEs calculated from nine planes near the SF are the same as the system SFEs. This, however, is not a SF range effect because nine planes would include all planes in systems.
- The non-correlation might be an illusion because it can be caused by H relocation between planes.
- ML is needed to explore the correlation between system SFEs and plane alloy compositions near SF.

SUMMARY

1. Extensive time-averaged MD simulations have been performed to study SFE in stainless steels.
2. SFE in alloys is not a single value, but rather a distribution due to local composition variations.
3. H can increase or decrease local SFE, but always significantly reduces the mean SFE of large systems (or many small systems), in agreement with experiments.
4. For H-free systems, local SFEs depend mainly on the two planes closest to SF. ML is needed to explore if local SFEs of H-containing system also depend mainly on alloy compositions of a few planes near SF.
5. A large database is already created for such ML studies.

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.