Development of Fe-Ni-Cr-H Interatomic Potential

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Five criteria of Fe-Ni-Cr potential

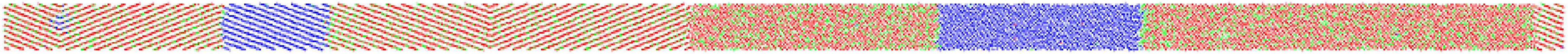
1. Give reasonable energy and volume for various compositions
2. Permit stable MD simulations of austenite
3. Prescribe well the elastic constants
4. Capture the correct stacking fault energy (γ_{sf})
5. Pass stringent MD validation tests

Five more criteria for adding H

1. Give good diffusion barriers in Fe, Ni, Cr
2. Prescribe well Fe-H, Ni-H, Cr-H energy trends
3. Capture correct swelling volumes in Fe, Ni, Cr
4. Match negative H-H energies from DFT
5. Pass stringent MD validation tests

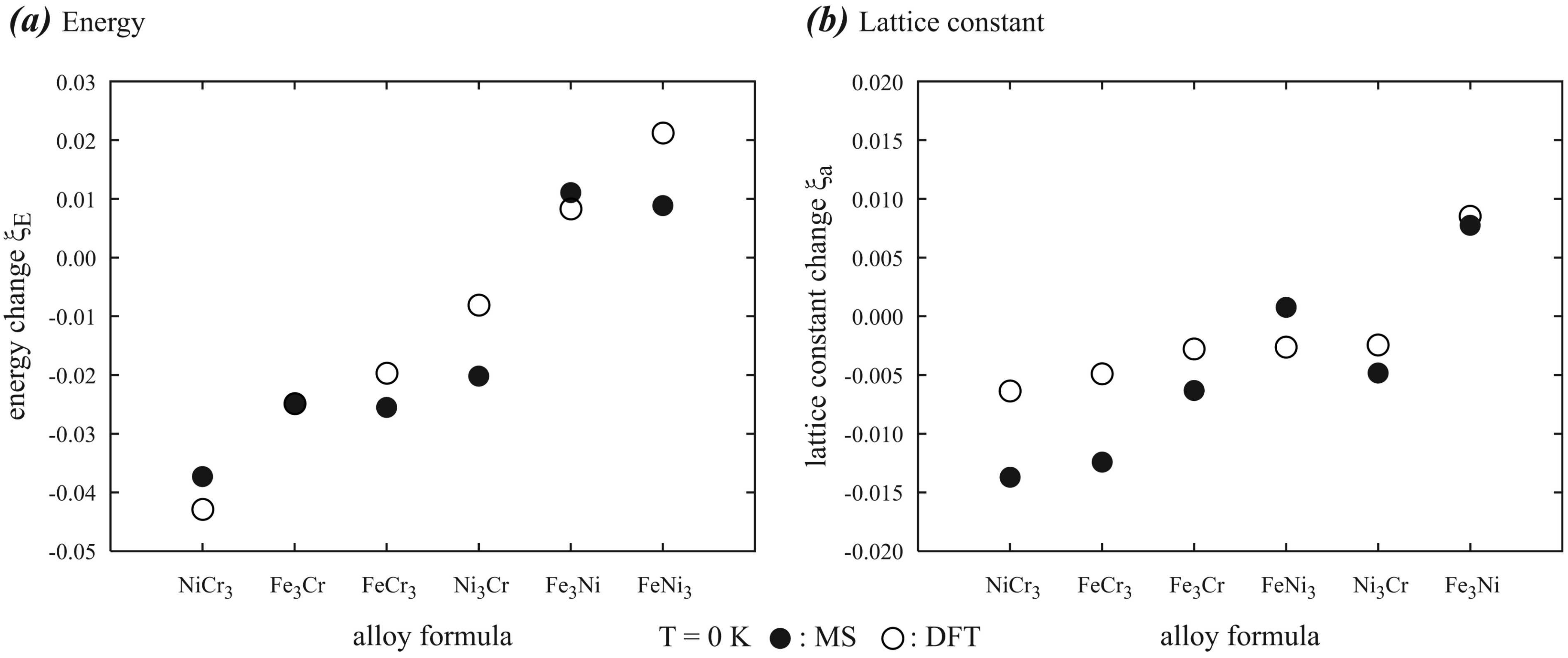
Status of literature Fe-Ni-Cr potentials

1. Our old potential (CALPHAD 1993, 17, 383) did not consider the four criteria
2. Smith and Was' potential (PRB 1989, 40, 10322) was fitted to effective atoms and did not consider stacking fault energy
3. The 2013 version of Bonny et al's potential (MSMSE 2013, 21, 085004) incorrectly predicts phase separation



4. The 2011 version of Bonny et al's potential (MSMSE 2011, 19, 085008) incorrectly predicts negative slope of stacking fault energy with Ni composition
5. Tong et al's potential (Mol. Sim. 2016, 42, 1256) incorrectly predicts large negative stacking fault energy (~ -200 mJ/m^2)
6. The 2018 version of Bonny et al's potential (MSMSE, 2018, 26, 065014) is based on the 2013 version

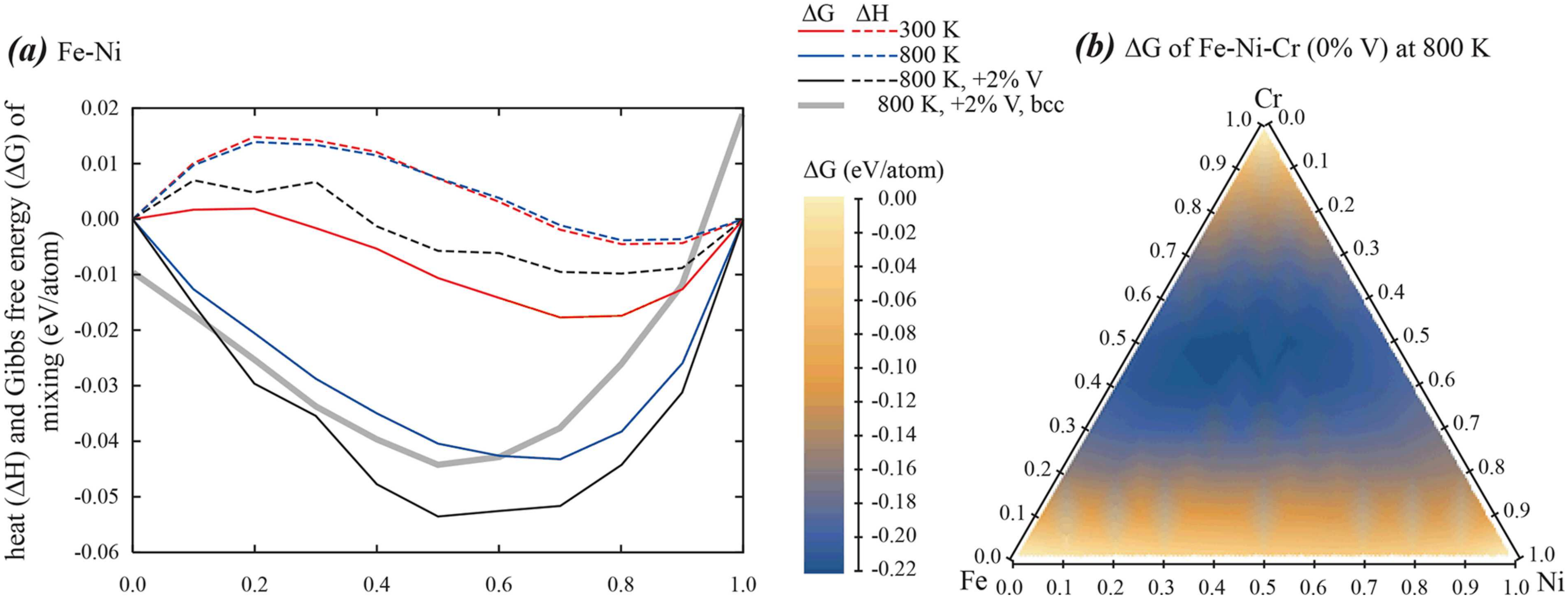
Fe-Ni-Cr criterion 1: Energy and volume trends



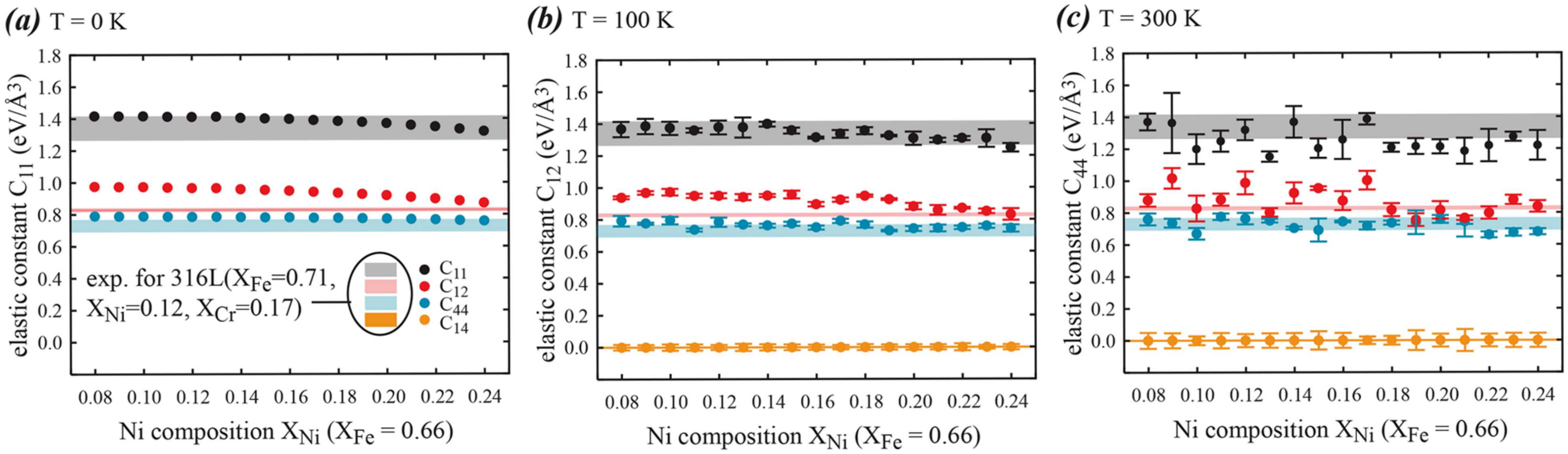
Calculated welling parameters for Ni and Cr in bcc Fe are 10% and 8% respectively, compared to 5% and 4% experimental values (King, J. Mater. Sci., 1, 79, 1966)

Fe-Ni-Cr criterion 2: Stable austenite

Overview of Gibbs free energy of mixing

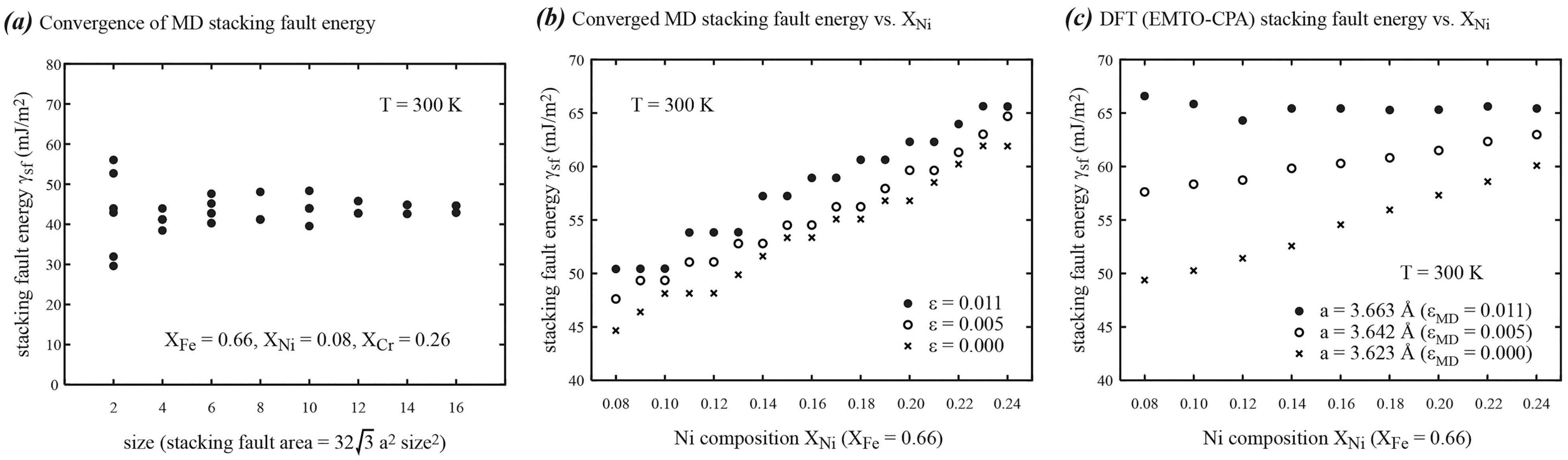


Fe-Ni-Cr criterion 3: Elastic constants



Experimental data for 316L from **(1)** Ledbetter, Ultrasonics 1985, 23, 9; **(2)** Bonny et al, MSMSE 2011, 19, 085008; **(3)** Bonny et al, MSMSE 2013, 21, 085004.

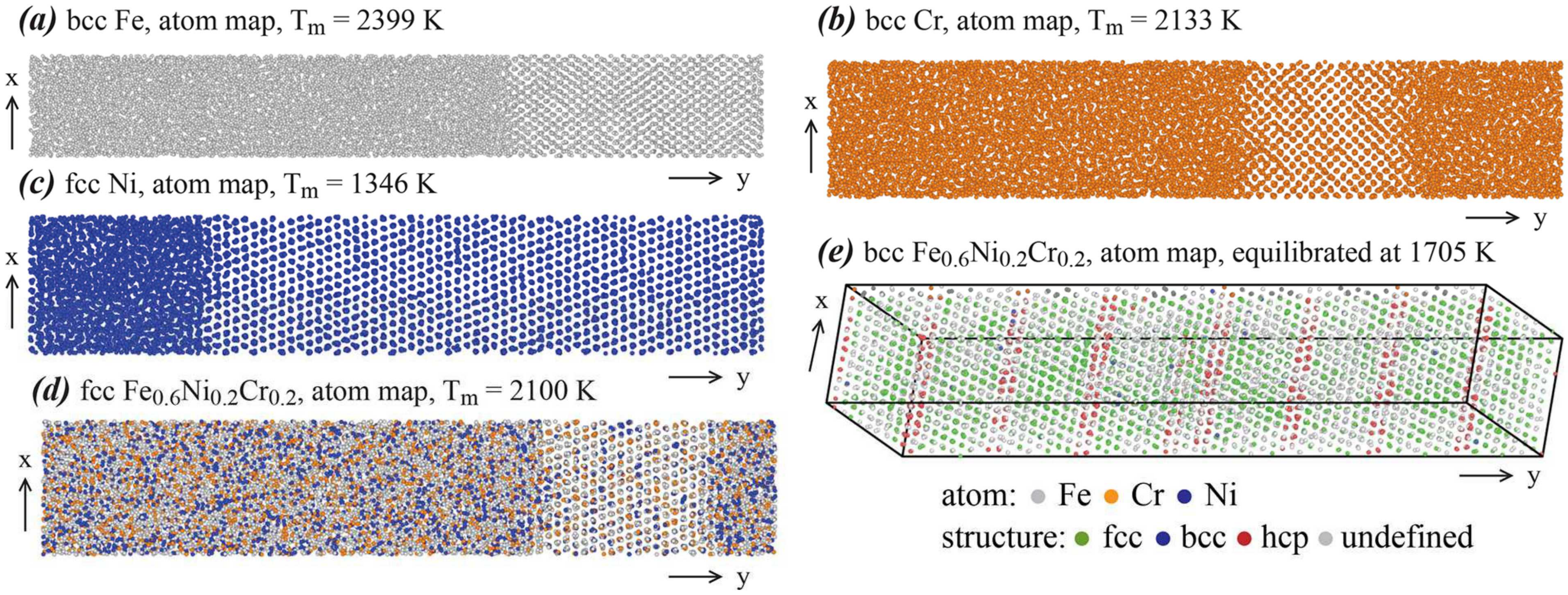
Fe-Ni-Cr criterion 4: Stacking fault energy



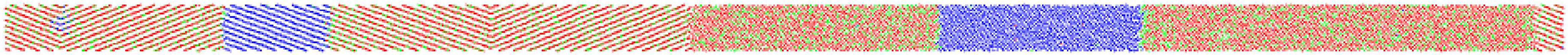
maximum area ~ 1000 nm^2

The predicted stacking fault energies match well with experimental results (see, for example, Vitos et al, PRL 2006, 96, 117210, and references therein).

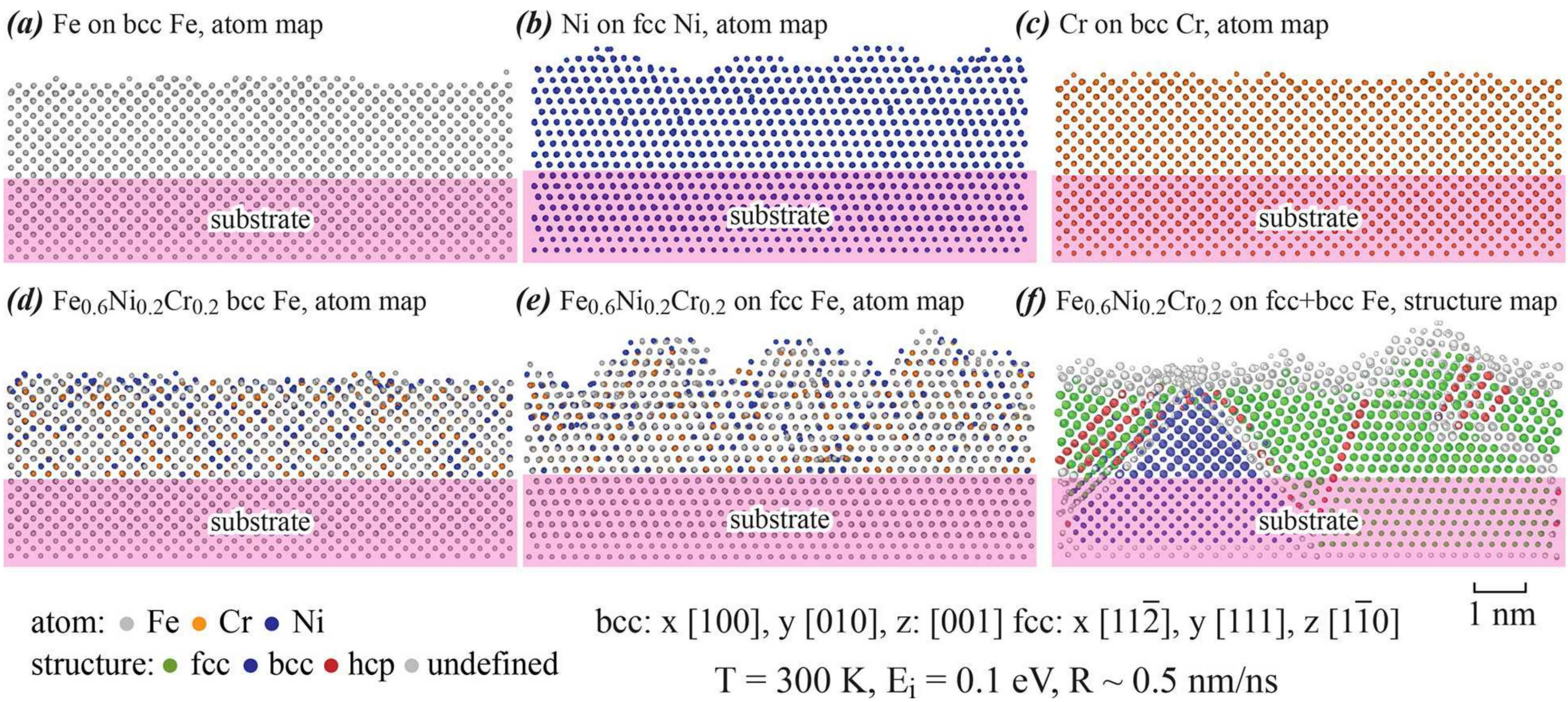
Fe-Ni-Cr criterion 5: Stringent MD melting tests



Note Bonny et al's 2013 version gives:

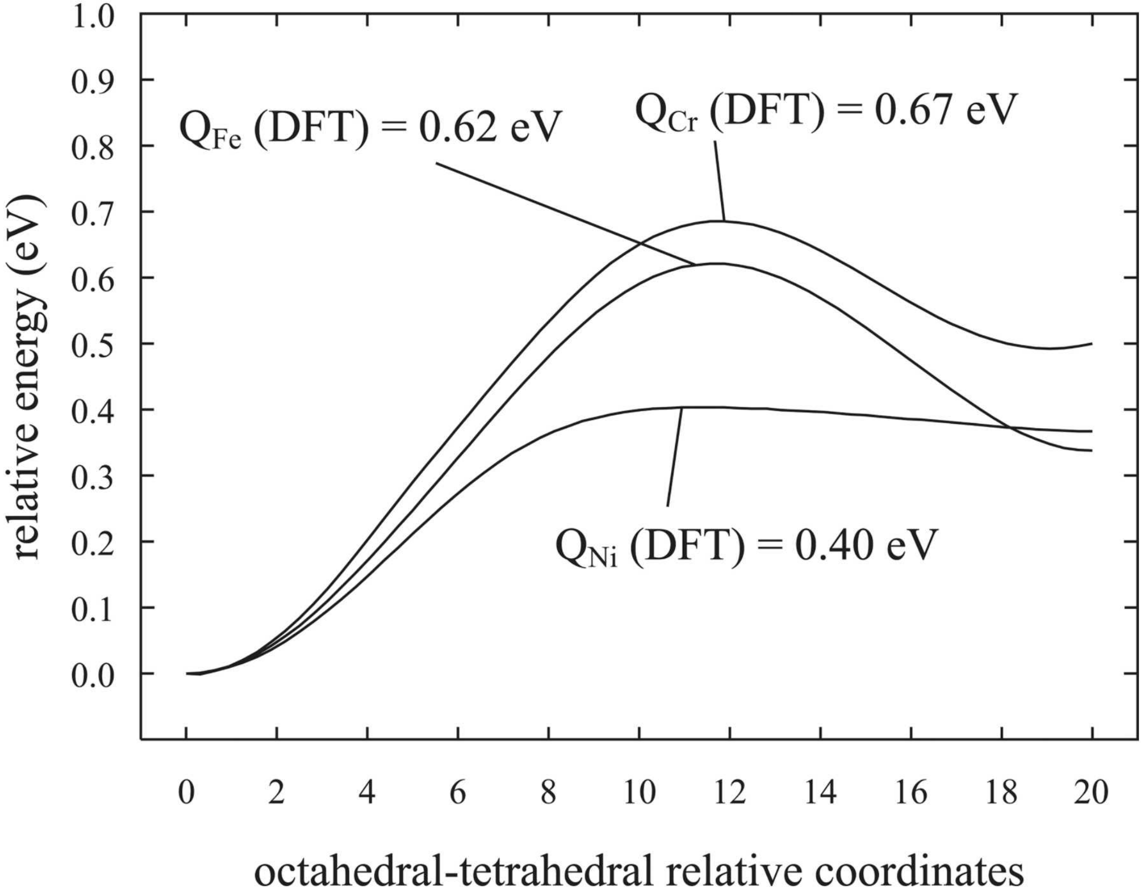


Fe-Ni-Cr criterion 5: Stringent MD growth tests

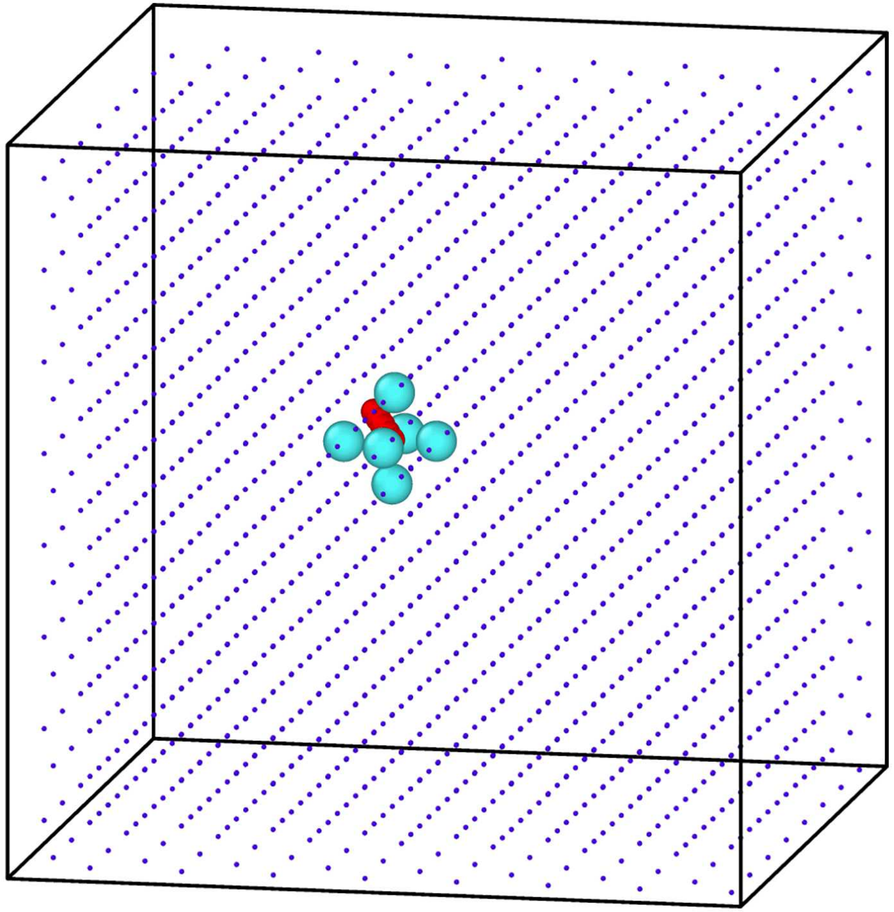


H criterion 1: Diffusion energy barriers

Diffusion barrier Q_M under local M environment. Local Cr assumes fcc Fe matrix, otherwise local and matrix atoms are the same



Configuration for calculation Q_{Cr}: Small blue: Fe; big blue: Cr; red: H3



H criteria 2-4: H swelling volume/energy trends in Fe, Ni, Cr, and H-H energy in Fe and Ni

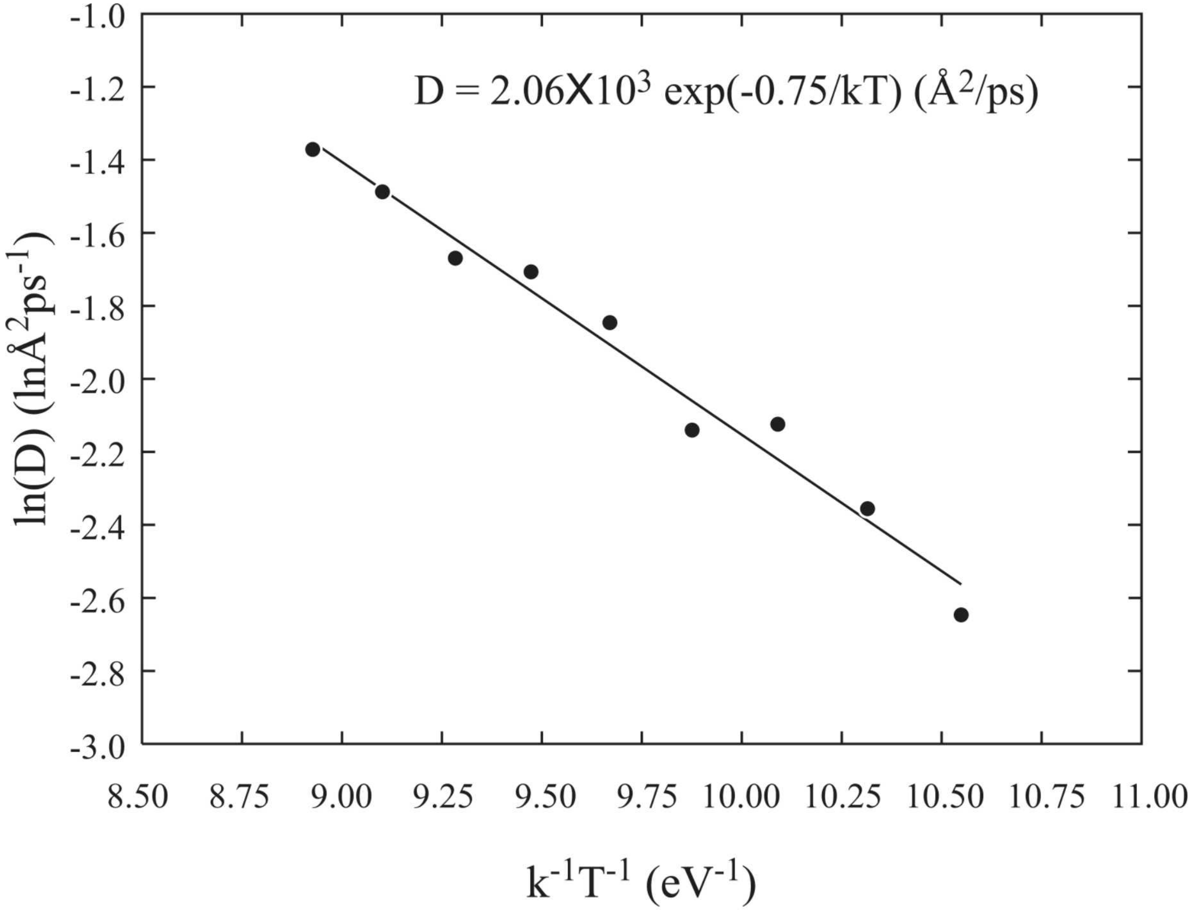
Table I. H swelling volume Ω_H, relative H binding energy under local M environment $\Delta E_{H(M)}$, and H-H interaction energy under local M environment $\Delta E_{H-H(M)}$. Matrix is either fcc Fe or fcc Ni

property	M = Fe (in fcc Fe)		M = Ni (in fcc Ni)		M = Cr (in fcc Fe)	
	MD	DFT	MD	DFT	MD	DFT
Ω_H (Å^3)	2.11	2.16	2.44	2.23	1.90	1.95
$\Delta E_{H(M)}$ (eV)	0.00	0.00	-0.19	-0.14	-0.36	-0.29
$\Delta E_{H-H(M)}$ (eV)	-0.015	-0.010	-0.053	-0.028[1]	-----	-----

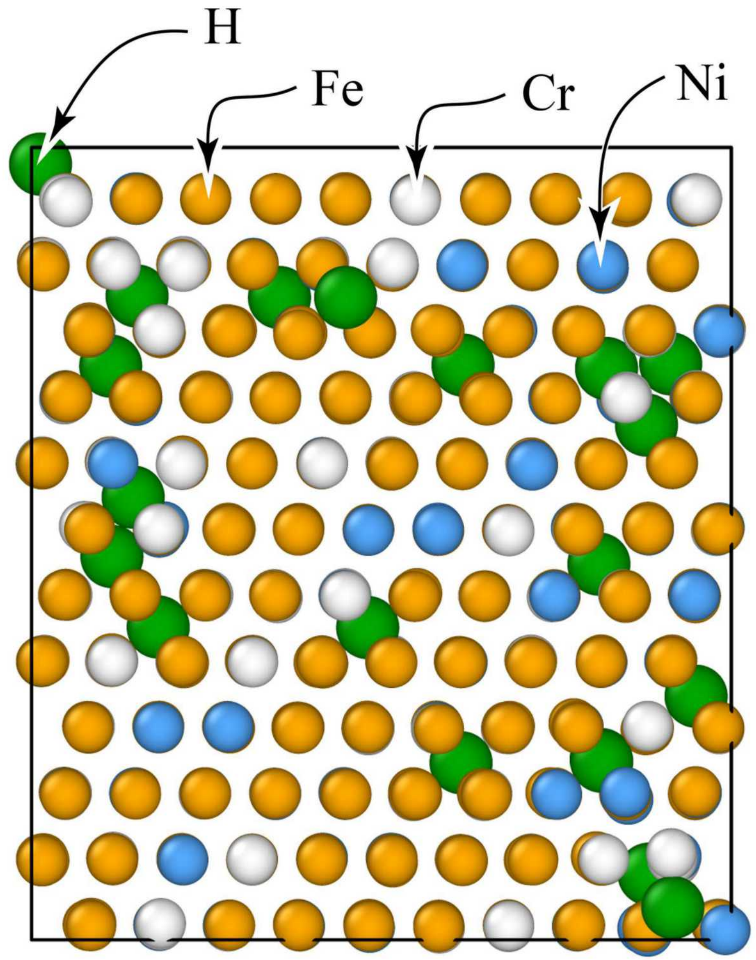
1. von Pezold et al, Acta Mater. 2011, 59, 2969.

H criterion 5: Stringent MD H diffusion simulations

Arrhenius derived from MD simulations



Configuration from MD



T = 1300 K, t = 23 ns

Conclusions

- Our Fe-Ni-Cr potential
  - Gives reasonable energy and volume for various compositions
  - Permits stable MD simulations of austenite
  - Prescribes well the elastic constants
  - Captures the correct stacking fault energy
  - Passes stringent MD validation tests
- Our H-metal potential
  - Gives good diffusion barriers in Fe, Ni, Cr
  - Prescribes well Fe-H, Ni-H, Cr-H energy trends
  - Captures correct swelling volumes in Fe, Ni, Cr
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  - Passes stringent MD validation tests