Upscaling from DFT to Interatomic Potential

2/16/2022

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Requirements Defined by Downscaling from Atomic Level

*First Order Requirements for EAM/MEAM Potentials (for **calibration**)*

- Lattice parameter: a_0
- Elastic Moduli: C_{11}, C_{22} (C_{11}-C_{22}/2: tetragonal shear modulus), C_{12}, C_{13}, C_{22}, C_{33}, and C_{44} (trigonal shear modulus)
- Cohesive Energy (heat of formation): E_C
- Volume: V_0
- Exponential Decay Factor for MEAM potential: α

*Objectives for Optimization of Parameters for EAM/MEAM Potentials (for **validation**)*

- Surface Formation Energies
- Generalized Stacking Fault Curve
- Vacancy Formation Energy
- Atomic Forces
- Lattice ratio: HCP c/a ratio
- Crystal energy differences: E_{fcc}-E_{hcp}
- Crystal energy differences: E_{bcc}-E_{hcp}

Cohesive Energies

$$E_{coh} = \frac{(E_{tot} - NE_{atom})}{N}$$

E_{coh}: cohesive energy of an atom

E_{tot}: total energy of the system consisting of N atoms

E_{atom}: total energy of an isolated atom

- Cohesive energy of an atom is defined as the heat of formation per atom when these atoms are assembled into a crystal structure

- When plotting the cohesive energy vs. the lattice parameter, the minimum of the cohesive energy curve determines the equilibrium lattice constant a_0

Joost et al. (2015)
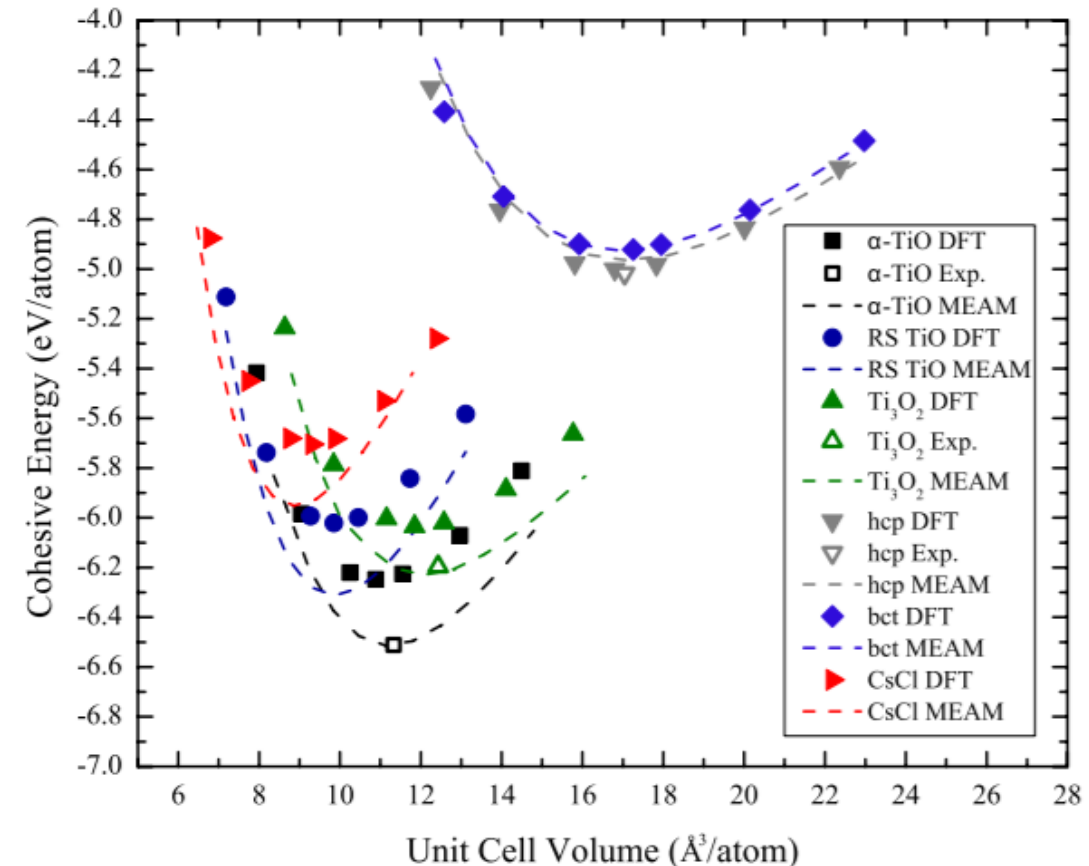
Elastic Constants

- Number of elastic constants varies in different crystal structures

- Hexagonal crystal have five independent elastic constants: C_{11}, C_{12}, C_{13}, C_{33}, and C_{44}

- Cubic crystals have three independent elastic constants: C_{11}, C_{12}, and C_{44}

- The elastic constants are calculated numerically by applying small strains to the lattice

Surface Formation Energies

$$\gamma = \frac{(E_{tot} - N\epsilon)}{A}$$

γ: Surface formation energy per unit surface area
E_{tot}: total energy of the system with a surface
N: number of atoms in the system
ϵ: total energy per atom in the bulk
A: surface area

Vacancy Formation Energies

$$E_{vac} = E_{tot}[N - 1] - E_{tot}[N]$$

E_{vac}: energy cost to create a vacancy
E_{tot}: total energy of the system with N atoms containing no vacancy
$E_{tot}[N - 1]$: energy of system containing a vacancy in its most stable bulk structure

Surface Adsorption Energies

$$E_{ads} = E_{tot} - E_{surf} - E_{atom}$$

E_{ads}: adsorption energy of a single adatom
E_{tot}: total energy of the structure with the adatom adsorped on the surface
E_{surf}: total energy of the surface without the adatom
E_{atom}: the energy of an isolated atom

Stacking Fault Energy

$$E_{sf} = \frac{E_{tot} - N\epsilon}{A}$$

E_{sf}: stacking fault formation energy per unit area
E_{tot}: total energy of the structure with a stacking fault
N: the number of atoms in the system
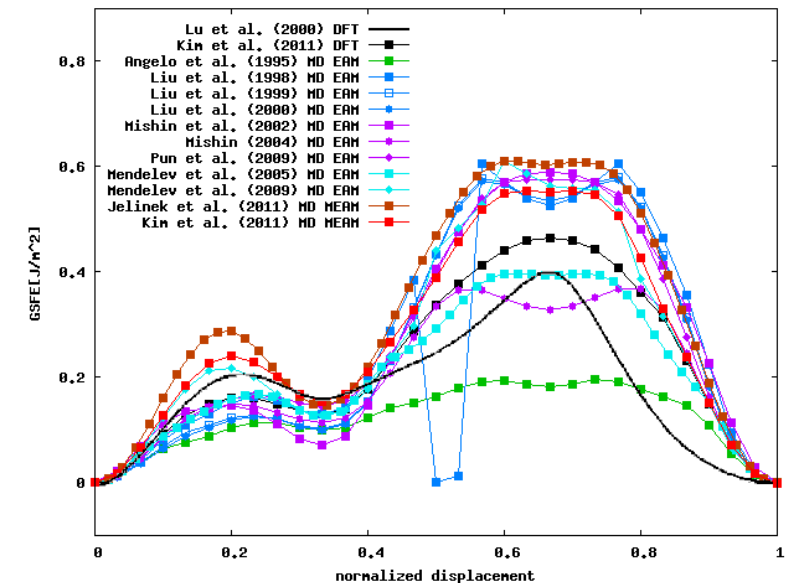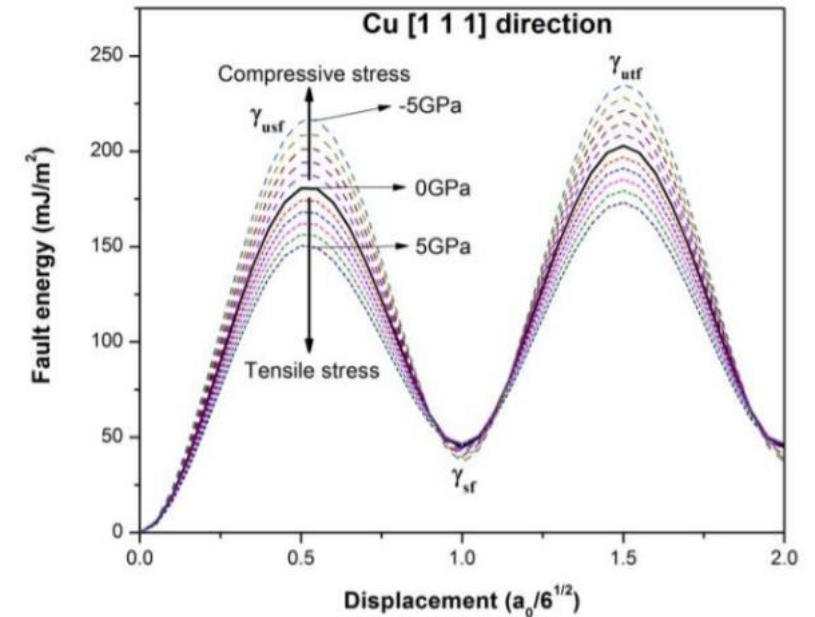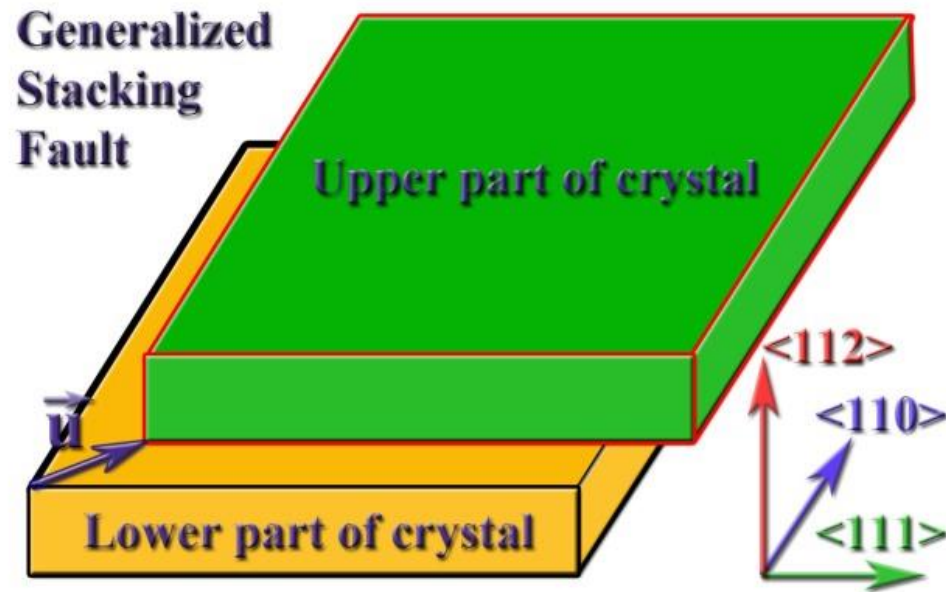ϵ: the total energy per atom in the bulk
A: the unit cell area that is perpendicular to the stacking fault

Generalized Stacking Fault Energy (GSFE) Curve

- A measure of the energy penalty between two adjacent planes during shear deformation in a specific slip direction on a given slip plane

- It represents the nature of slip and involving the stable (intrinsic, local minima) and unstable (local maxima) stacking and twin fault energies

- The GSFE curve and the associated energy properties can be used to model a vast number of phenomena linked to dislocations, plastic deformation, crystal growth, phase transition and twin–twin interactions (Shang et al., 2014)

- The nature of slip in crystalline metals cannot be described in terms of an absolute value of the stacking fault energy

- A correct interpretation requires the GSFE curve invoving both stable and unstable stacking fault energies

- GSFE is a key parameter to determine the structure and mobility of dislocation

Generalized Stacking Fault Energy (GSFE) Curve

Zhang et al. (2015)

Kim & Horstemeyer (2012)