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Bridging the Gap
–
Multi-scale modelling project with an emphasis on atomistic simulations

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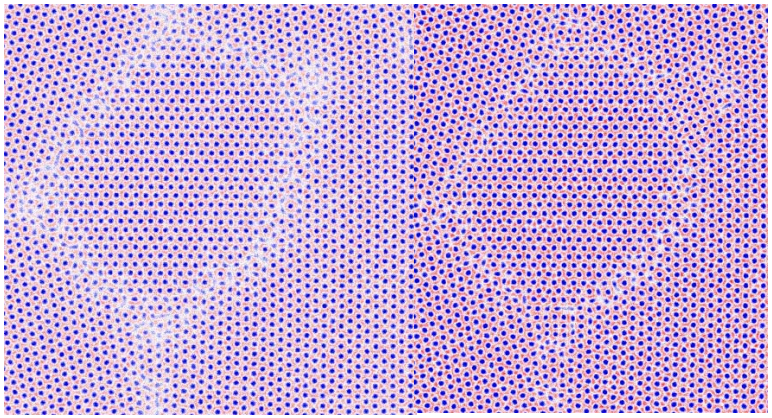
Modelling Across Different Length Scales

Atomistic:
$10^{-9} – 10^{-10}$ m

Microstructure evolution due to motion of atoms

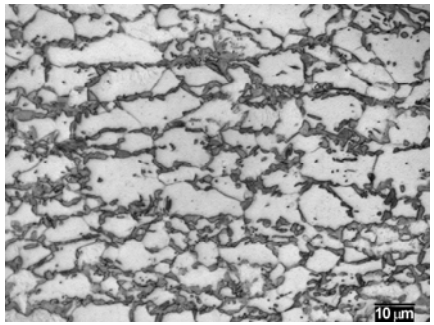


Density Functional Theory
Molecular Dynamics

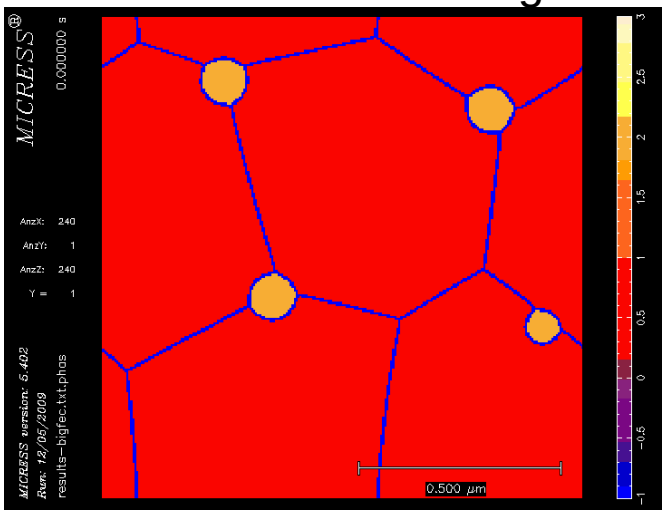
Phase Field Crystal

Mesoscale:
$10^{-6} – 10^{-4}$ m

Scale of microstructure

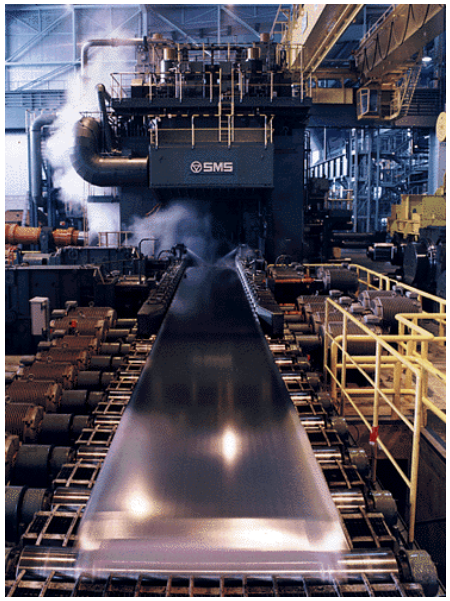


Phase Field Modelling



Macroscale:
0.01 – 10 m

Size of sheet metal



Process Models

Unknown Quantities

Mobilities and Solute Drag parameters

Adjustable parameters → M , D_b/δ and E_o

Can we determine all or some of these parameters from atomistic simulations?

- **M, Mobility of pure interface** (Molecular Dynamics)
- $D_b=D_o\exp(-Q_b/kT)$, Diffusivity of solute across interface (Molecular Dynamics?)
- **Q_b, Activation energy of interfacial solute diffusion** (Density Functional Theory)
- **E_o, Binding energy of solute to interface** (Density Functional Theory)

Project Flow: Length and Time Scales

Atomistic:

DFT (density functional theory): ab-initio calculation of binding (E_o) and activation energies (E_A) of solutes at α-γ interface

MD (molecular dynamics): Use DFT results to build suitable potentials for simulations of mobility (**M**) of α-γ interface
Note: Time scale of atomic vibrations, i.e. approx. 10 ns

Mesoscale:

PFM (phase field model): Use DFT/MD/PFC (c_2) results for binding energy (E_o), interfacial diffusion (D_b) and mobility (**M**) to simulate **solute drag** and overall transformation kinetics

PFC (phase field crystal): Provide linkage from atomistic to continuums modelling using MD length scale and PFM time scale, translate interaction potentials to two-point correlation function (c_2)

Macroscale:

JMAK (Johnson-Mehl-Avrami-Kolmogorov): Translate PFM **solute drag** model into suitable **JMAK rate parameters** for overall **transformation model**

Validation Experiments: **Validate transformation model** with experimental data

Density Functional Theory Studies

Hao Jin, Ilya Elfimov and Matthias Militzer

UBC

THE DREAM

Tell the computer how many and what kind of particles one has in a problem of interest and get the exact solution based solely on this information.

Quantum Mechanics – theory to provide this solution

Schrödinger equation: $\hat{H}\Psi_i = E_i\Psi_i$

BUT: Many body effects (electron-electron interaction) are difficult/impossible to treat even numerically (solutions just available for small systems)

THUS:

Need suitable approximations → Density functional theory (DFT)

DFT in a nutshell

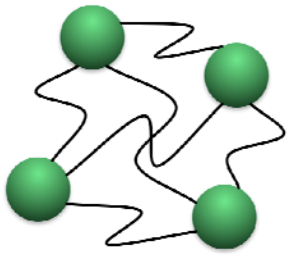
Hohenberg and Khon :

$$\rho(\vec{r}) \xrightarrow{F(\rho(\vec{r}))} E_{Total}$$

Electron density — Total energy

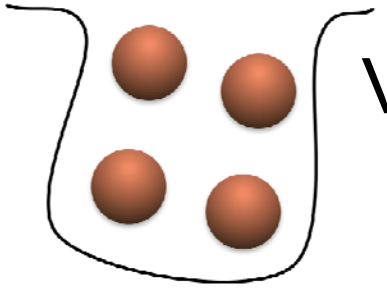
If functional *F* is known, one can immediately find the total energy of the system for any given electron density distribution.

Khon and Sham:



Replace interactions with an effective potential

$\rho_{int} = \rho_{nonint}$



Since ρ is the same, the total energy must be the same too.

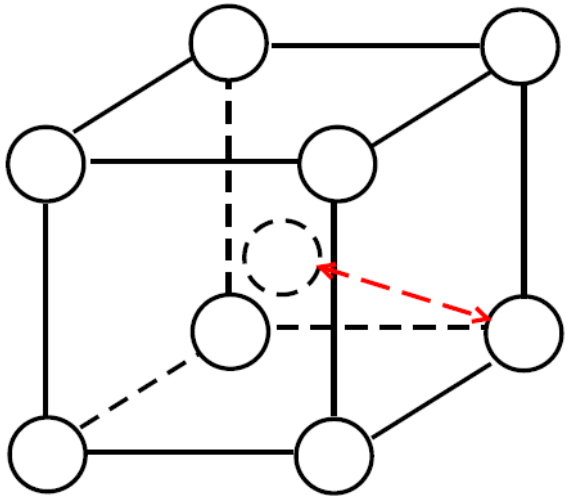
Need to find approximations for V_{eff} using theory of interacting electron gas (LDA, GGA).

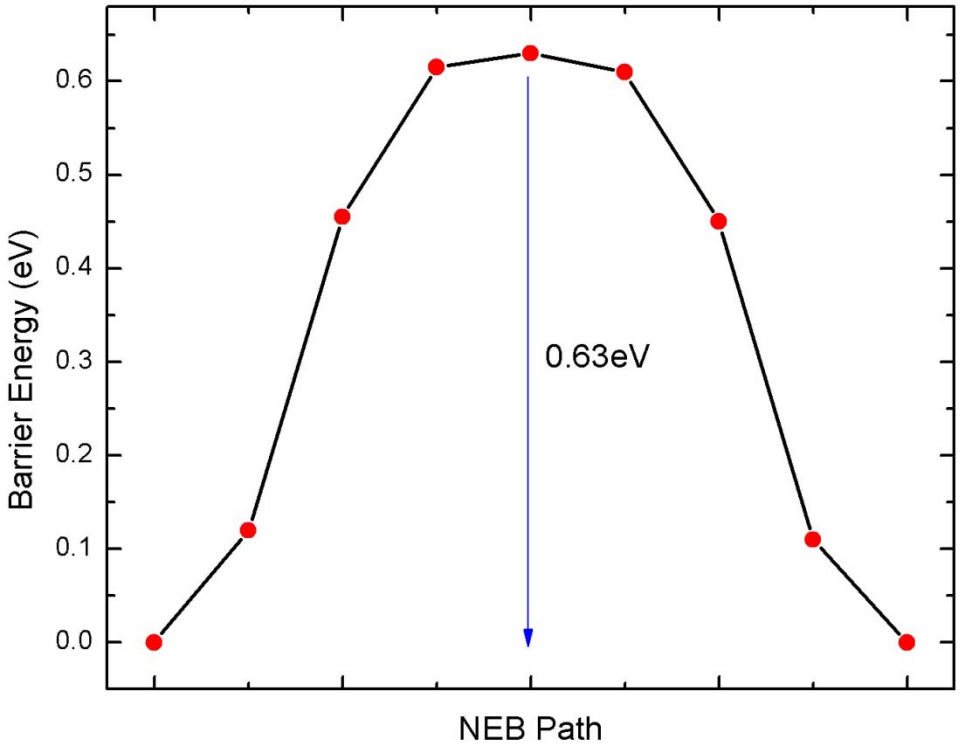
Note: Ground state theory – T = 0 K, can consider ~ 100 atoms

Self Diffusion in bcc Fe

VASP – commercial DFT code using pseudo-potentials

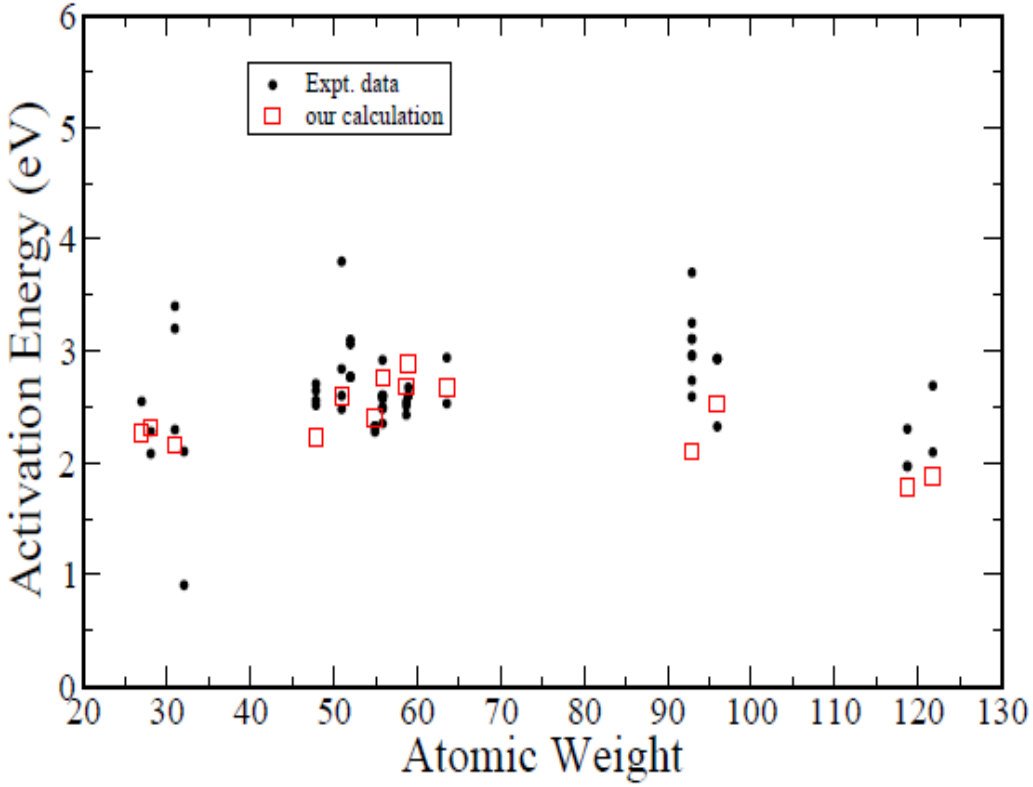
Supercell size: 3x3x3 (54 atoms)
Migration energy:
E_b=0.63 eV
Vacancy Formation energy:
E_{vf}=2.13 eV
Activation energy
$E_A=E_b+E_{vf}$=2.76eV





First-neighbor diffusion of the vacancy. One vacancy located in the centre diffuses along the red line to the corner of the cubic cell.

Substitutional Diffusion in bcc Fe



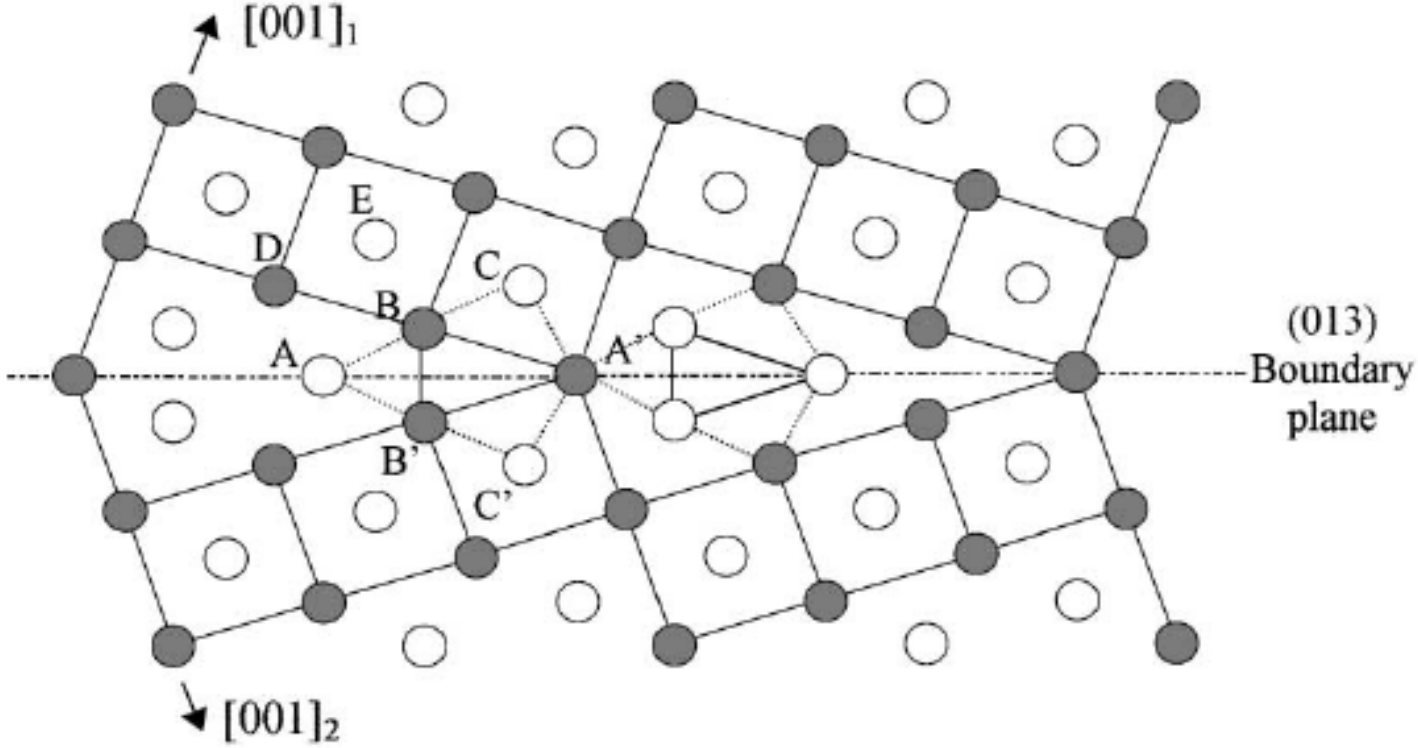
	Evf	Eb	Ea (eV)
Al	1.85	0.41	**2.26**
Si	1.88	0.43	**2.31**
P	1.82	0.34	**2.16**
Ti	1.93	0.30	**2.23**
Fe	2.13	0.63	**2.76**
Co	2.21	0.68	**2.89**
Ni	2.07	0.61	**2.68**
Nb	1.80	0.29	**2.09**
Mo	2.02	0.50	**2.52**
Sn	1.45	0.33	**1.78**
Sb	1.44	0.44	**1.88**

Substitutionals at Grain Boundaries

Consider Special Grain Boundaries

- boundaries with special properties, e.g. low energy
- finite fraction of lattice sites coincide between the two lattices $\rightarrow$ defines coincident site lattice (CSL).
- boundary with high density of lattice points in a CSL expected to have special properties
- special boundaries with high degree of symmetry can reasonably be considered in DFT (rather small calculation domains)

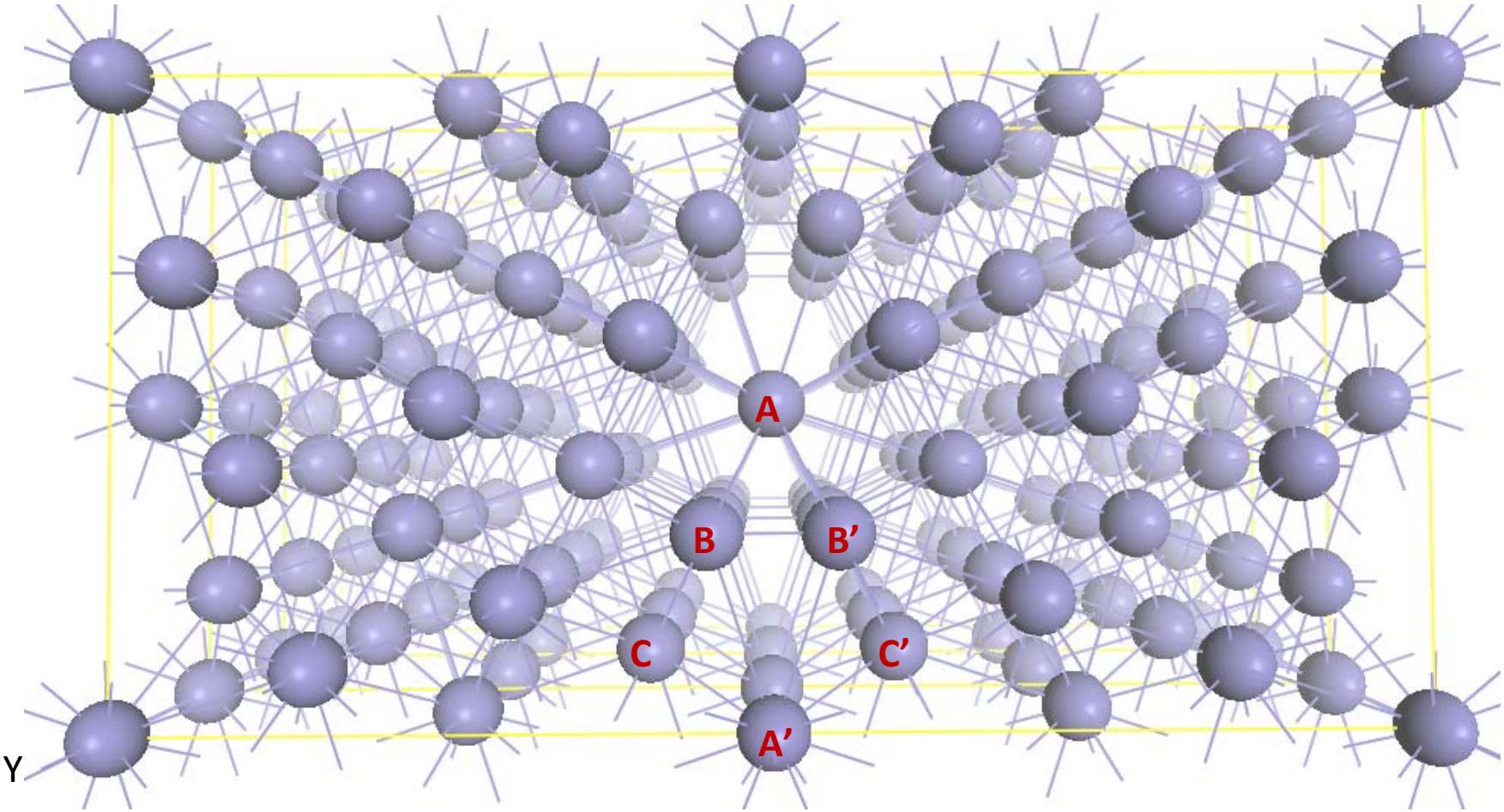
Σ5 [001] {013} Tilt Grain Boundary



The structure of the Σ5 [001] {013} tilt GB in bcc Fe. White circles and grey circles represent the ABAB… stacking sequence of the atomic planes perpendicular to the rotation axis. This boundary contains a stack of capped trigonal prisms (CTPs): ABCA'C'B' and has a mirror symmetry with respect to the (013) boundary plane.

Σ5 [001] {013} Tilt Grain Boundary

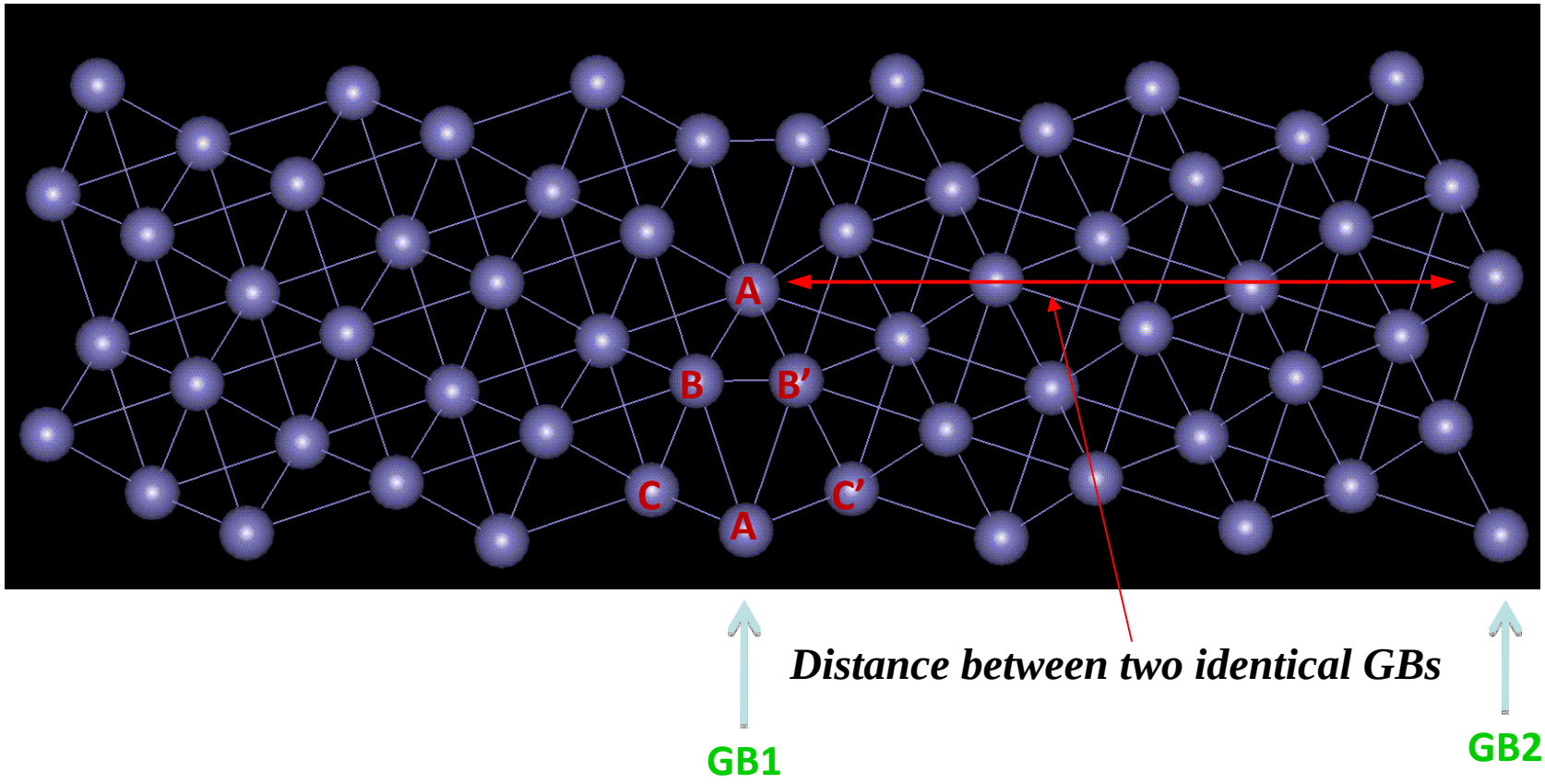
Perspective View



The shallow balls represent the next layers. Three yellow grids represent three layers in x direction

Σ5 [001] {013} Tilt Grain Boundary

One periodic supercell with two identical grain boundaries

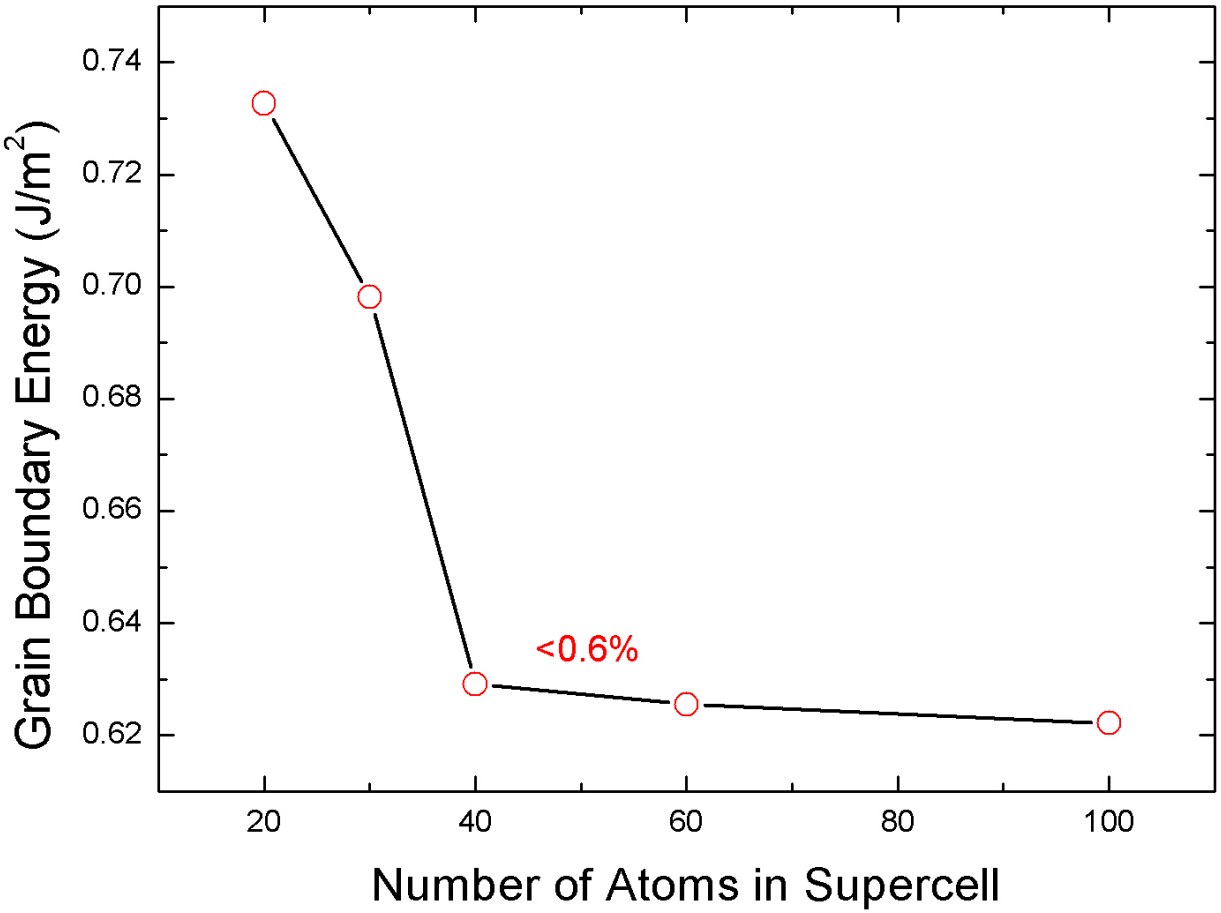


Grain Boundary Energy

$$\Delta E = \frac{1}{2}\left(E - E_{Bulk}\right)$$

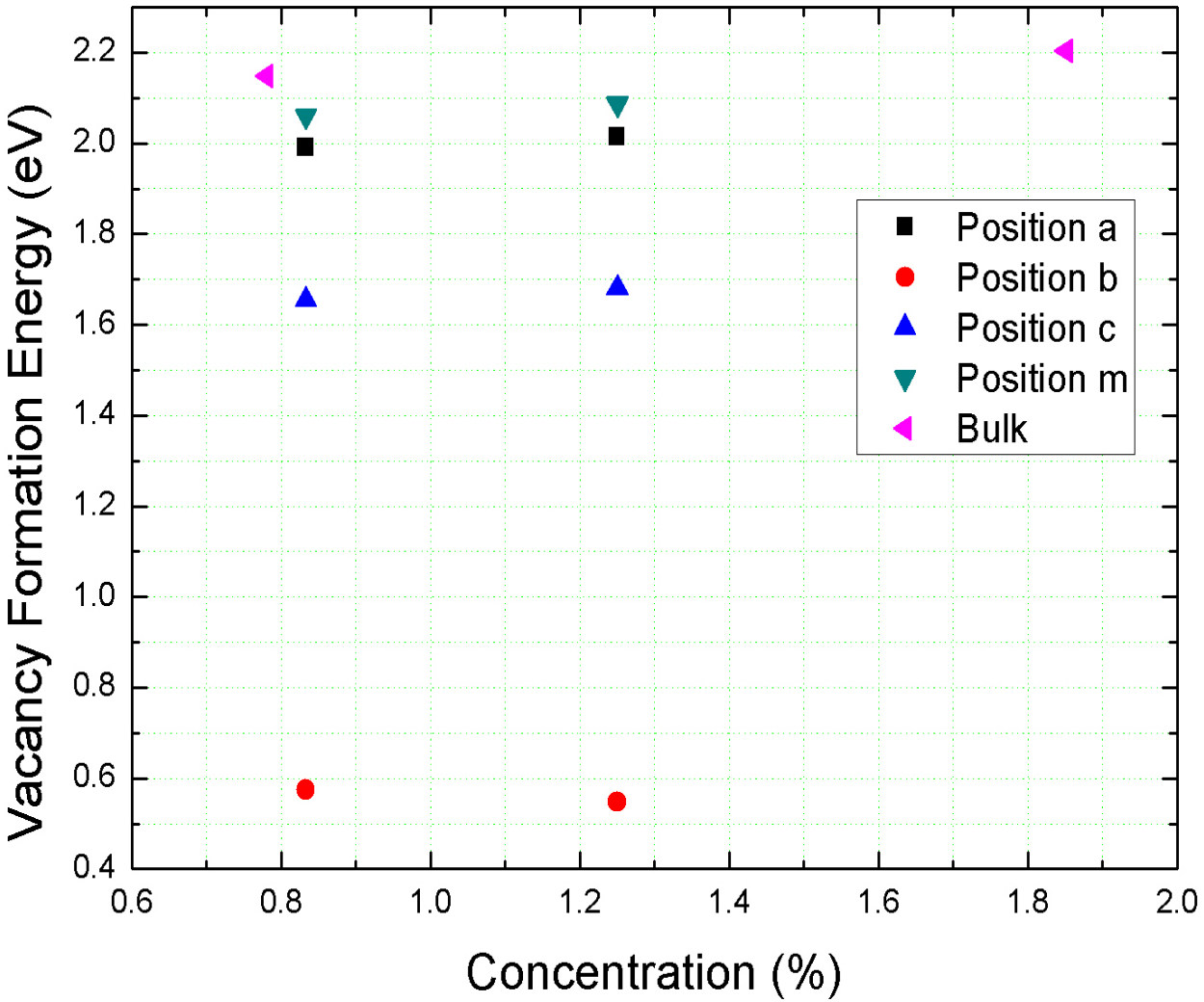
E total energy of supercell with grain boundary

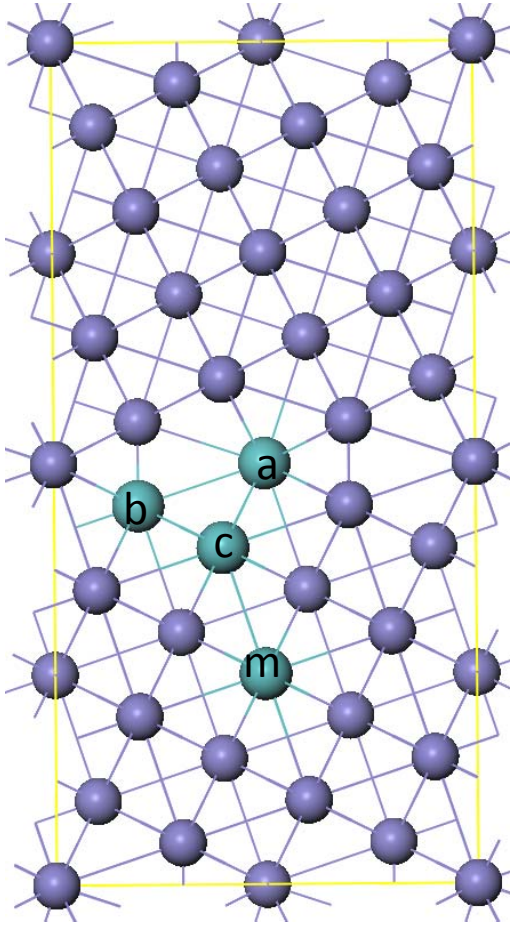
E_{Bulk} total energy of supercell without grain boundary



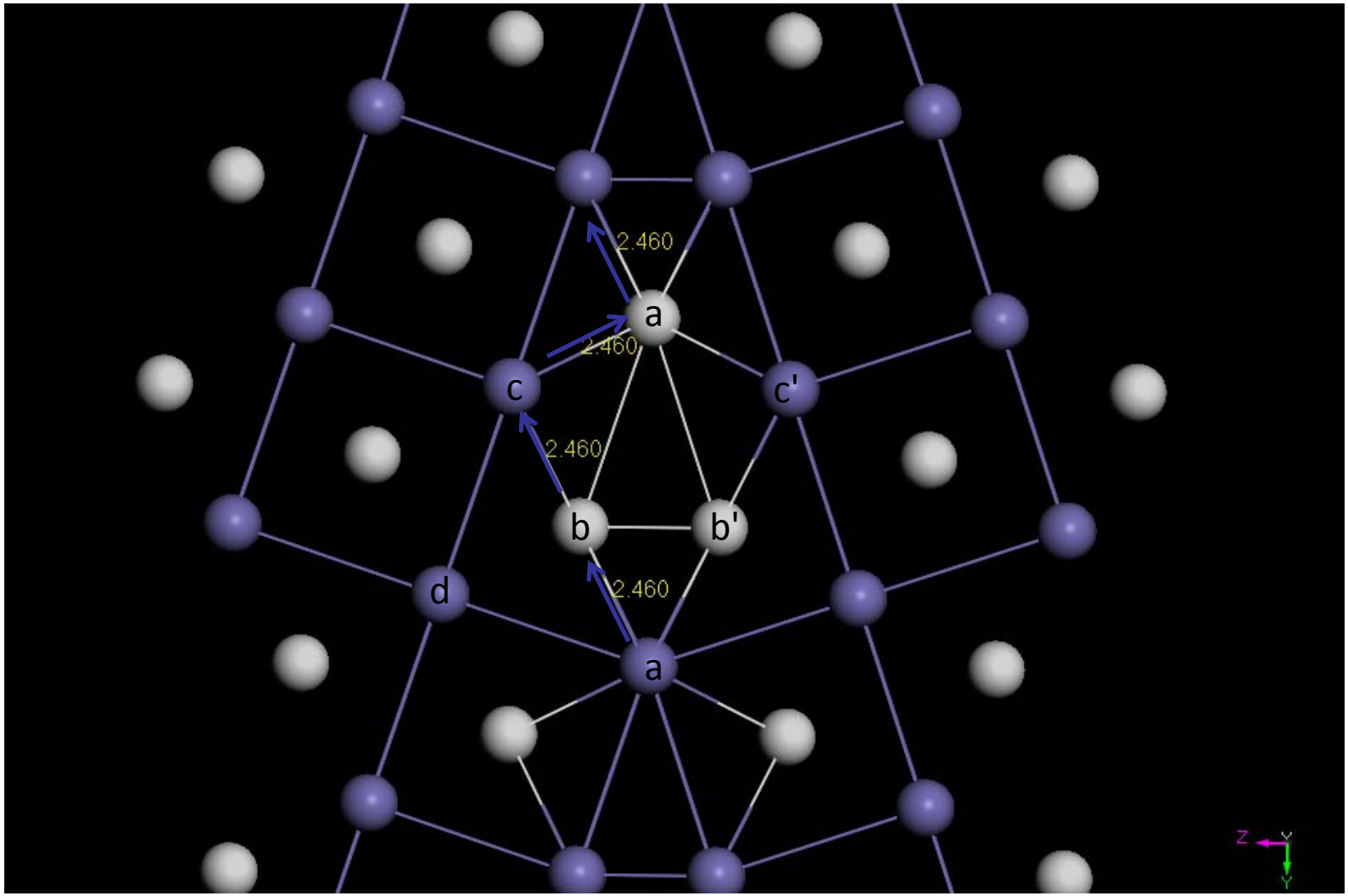
0.62 J/m^2

Vacancy Formation Energies (eV)

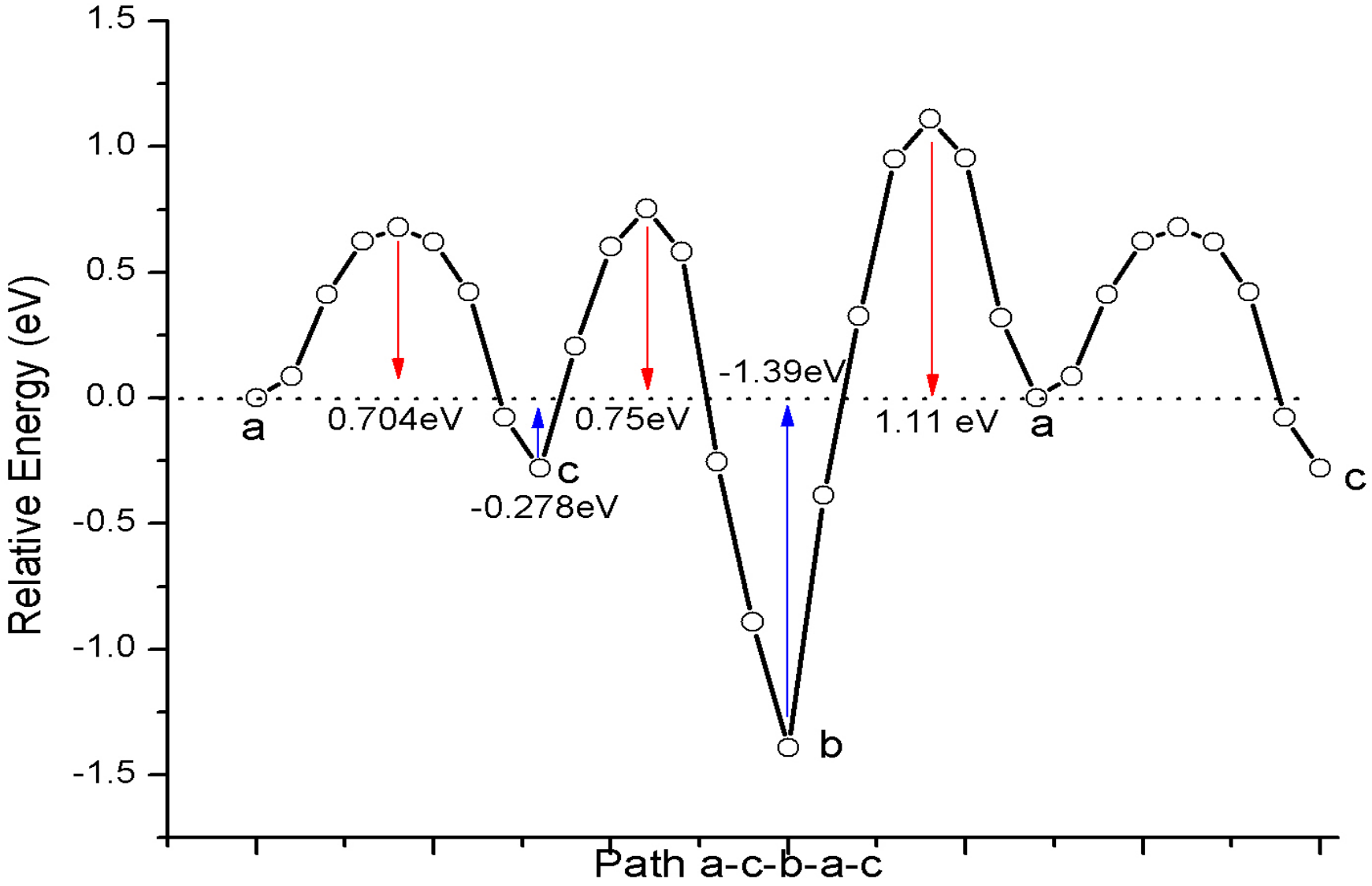




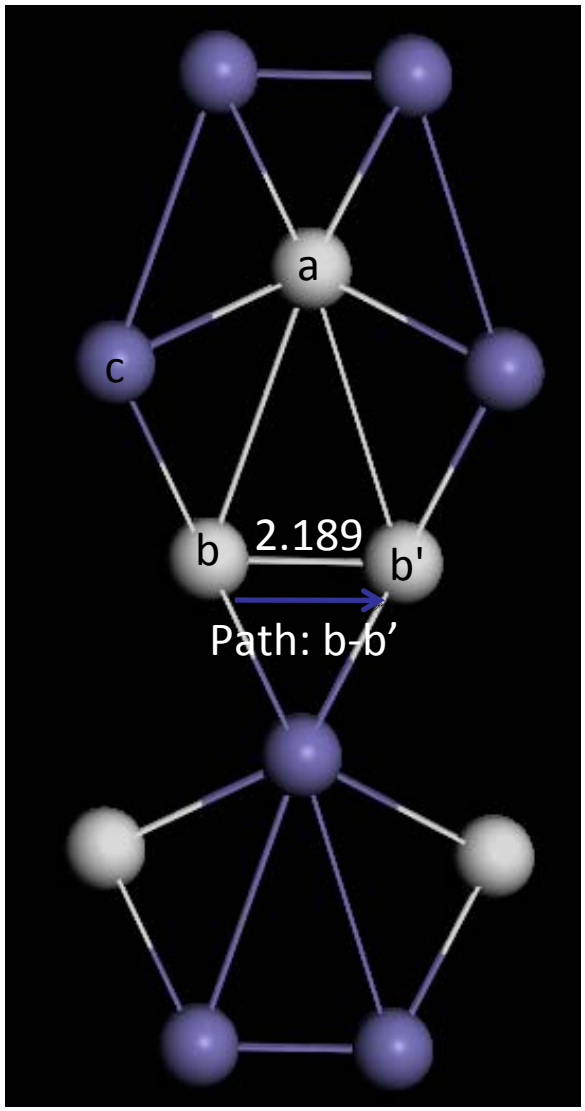
Vacancy-diffusion in Σ5 Tilt GB

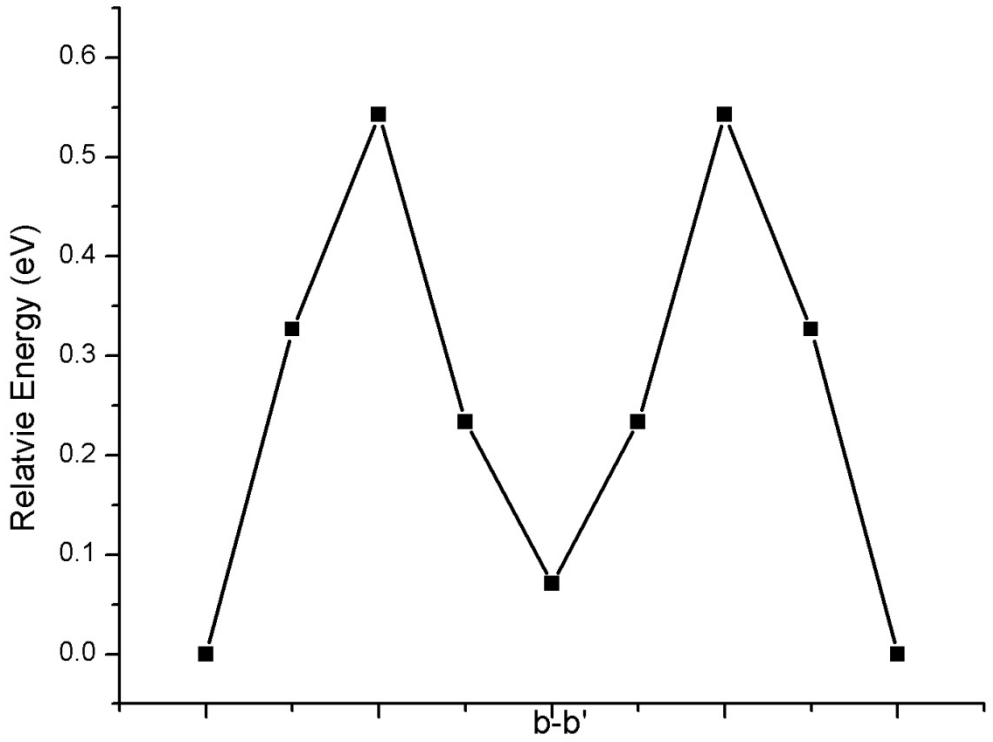


Vacancy-diffusion: a-c-b-a-c



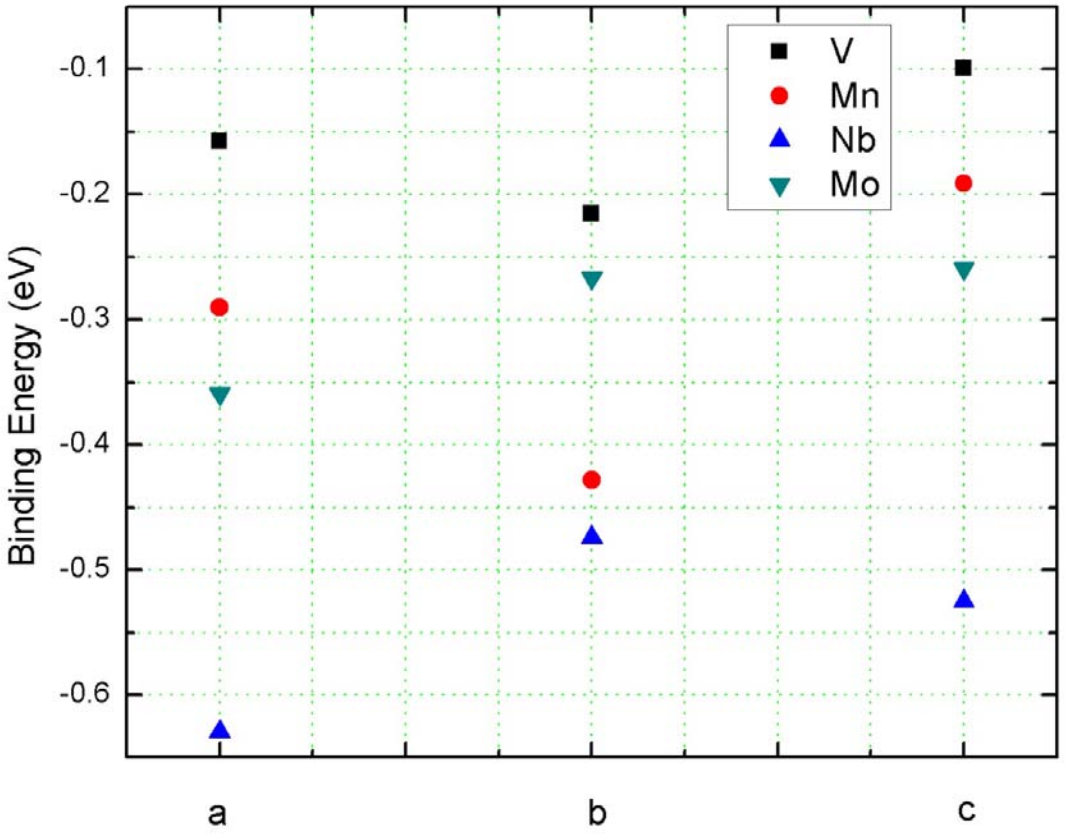
Vacancy-diffusion across Σ5 Tilt GB

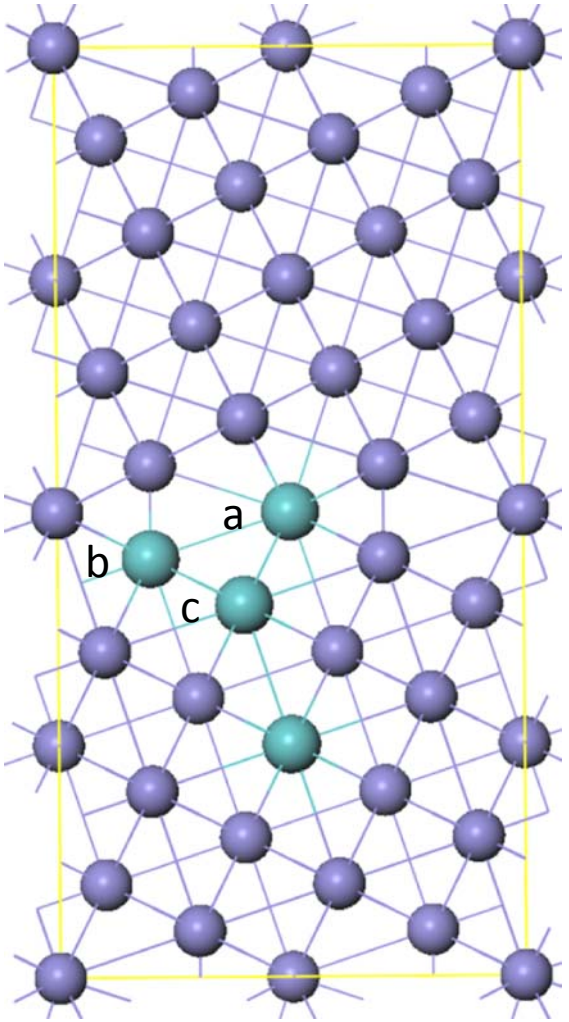




In this path, the energy barrier is 0.55 eV

Binding Energies of Substitutionals





Nb with higher binding energy compared to Mo, Mn and V
→ stronger interaction of Nb with grain boundaries
→ different site preferences for different solutes (Nb, Mo on a and Mn, V on b)

Future Work and Challenges

Determine activation energies for grain boundary diffusion of substitutional solutes

Determine binding and activation energies of substitutional solutes in the presence of carbon and/or other solutes

Develop kinetic Monte Carlo code to simulate grain boundary diffusion

Analyze magnetic state of austenite with DFT simulations (required to propose suitable assumptions for simulations of austenite-ferrite interface)