Atomistic modelling of oxygen solute hardening in titanium alloys.

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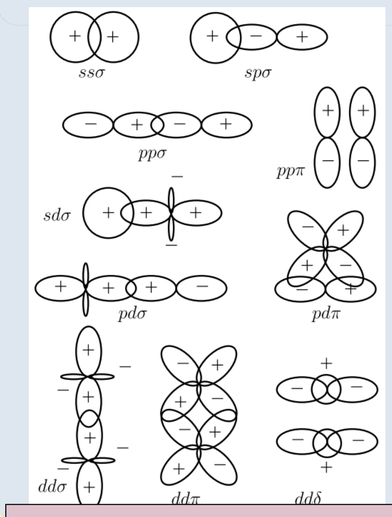
Screw dislocations control plasticity in titanium.

- ***Solute-hardening is not well understood on an atomistic scale.***
- ***Ab initio quantum mechanics is too computationally expensive.***
- ***Tight-binding approximation is quantum mechanical yet less expensive.***
- ***We have made a tight-binding model for titanium with which we can investigate atomistic mechanisms for oxygen solute-hardening.***



Tight-binding models need parameters.

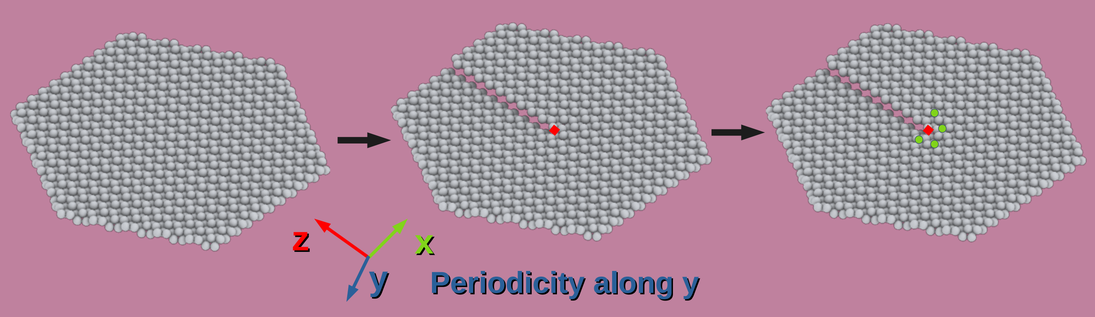
- ***Overlaps between atomic orbitals of atoms are parameters.***
- ***This titanium model is d-orbital only.***
- ***Ab initio Density Functional Theory (DFT) calculations and empirical quantities are fitted to.***
- ***Particle swarm algorithm used for fitting.***
- ***Validation achieved by comparison of:***
  - ***Lattice wave dispersion (phonons).***
  - ***Generalised stacking fault energy surfaces.***
  - ***Dislocation core structure.***
  - ***Dissolution/vacancy formation energies.***

Results of Fitting

Quantity	Units	TB model	Target
a_α	[bohr]	5.52	5.57
c/a	ratio	1.571	1.587
C_{11}	[GPa]	175.3	176.1
C_{33}	[GPa]	195.5	190.5
C_{44}	[GPa]	59.6	50.8
C_{12}	[GPa]	70.2	86.9
C_{13}	[GPa]	67.5	68.3

Method

- ***Create dislocation in cell.***
- ***Put oxygen into different sites (octahedral) near core.***
- ***Relax cell to see how the core structure changes.***

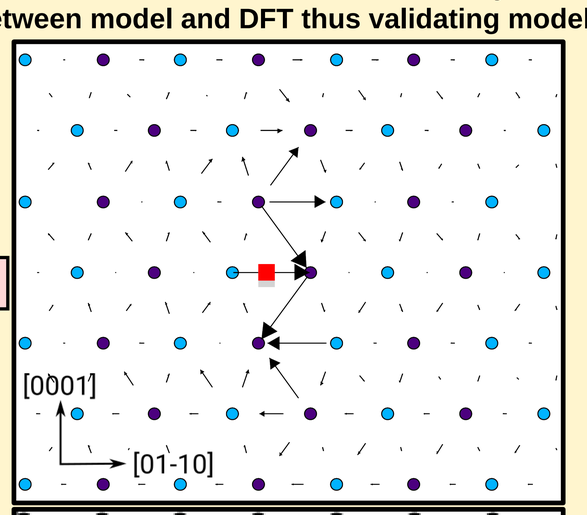


Dislocation Core Structure

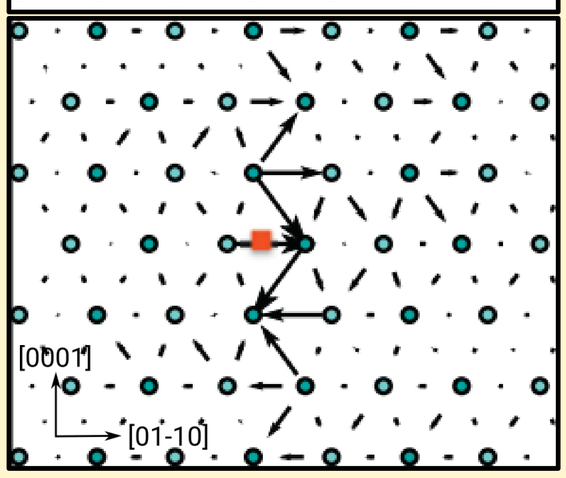
Differential Displacement maps of screw dislocation core upon relaxation in tight-binding (TB) and Density Functional Theory (DFT / a*b initio*).

- **Arrows denote out-of-plane displacements.**
- **An arrow joining two columns corresponds to displacement by a full Burger's vector. Position of elastic centre of dislocation core is marked by the red square.**
- **Good agreement between model and DFT thus validating model.**

Tight-binding



DFT [1]

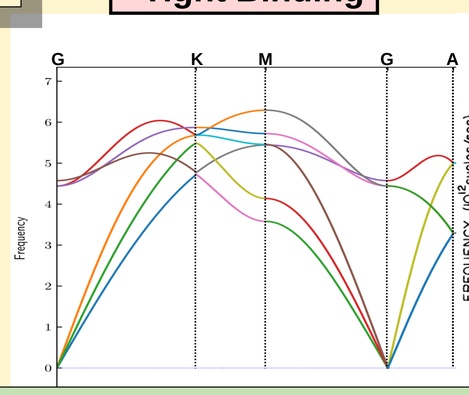


Validation Tests

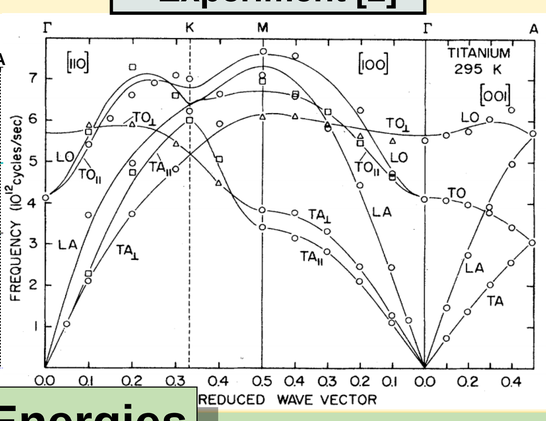
Quantity	Units	TB model	Literature
$E_{vacancy\ formation}$	[eV]	1.01	1.27 [Exp. Hashimoto (1984)] 1.95 [DFT Angsten (2013)]
$\Delta E_{solution}$(tetra. - octa.)	[eV]	0.80	1.20 [DFT Kwasniak (2013)]

Phonons

Tight Binding



Experiment [2]

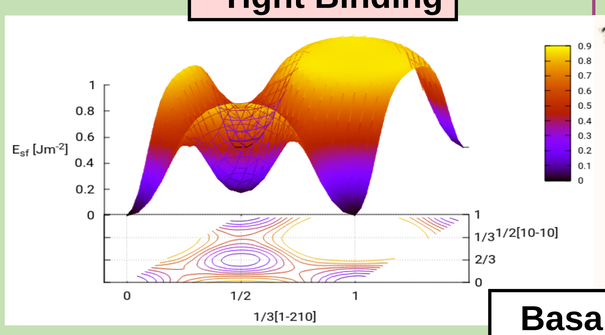


Generalised Stacking Fault Energies

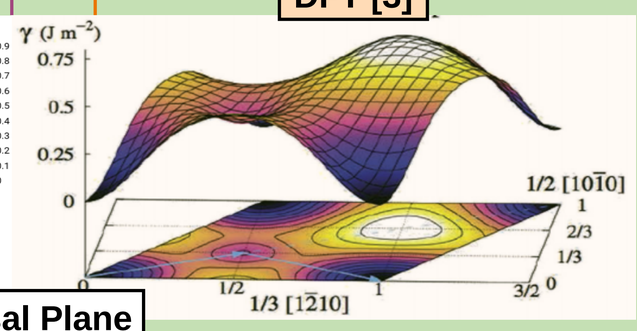
Gamma surfaces are plots of the excess energy of a faulted lattice, compared to an unfaulted one, with respect to fault vector.

- ***Minima show areas where stable stacking faults occur.***
- ***These predict possible dislocation dissociations in the model.***

Tight Binding

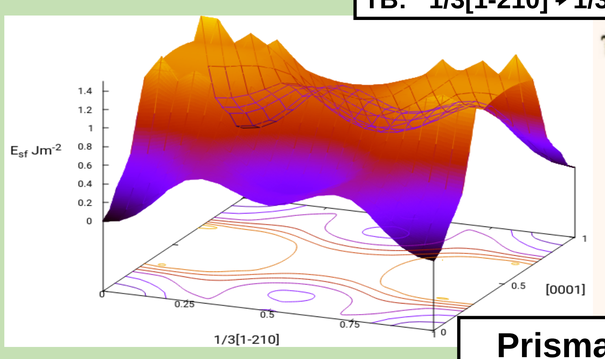


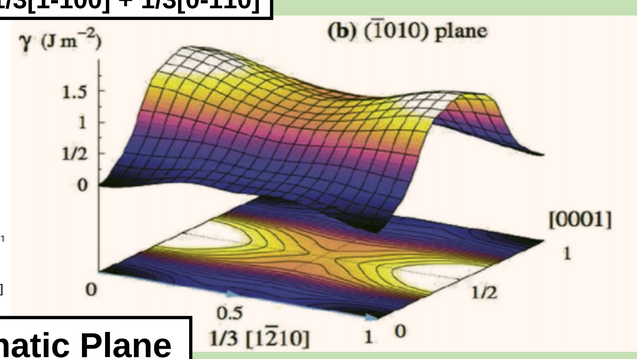
DFT [3]



Basal Plane

Predicted Splitting:
DFT: 1/3[1-210] → 1/3[1-100] + 1/3[0-110]
TB: 1/3[1-210] → 1/3[1-100] + 1/3[0-110]

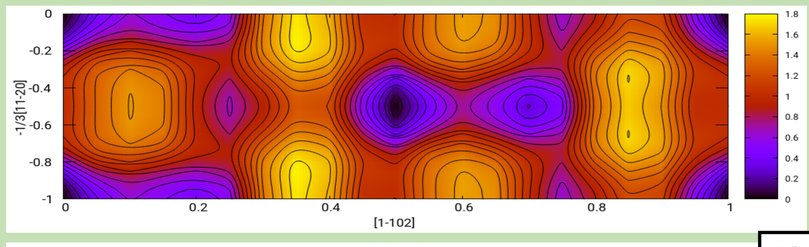




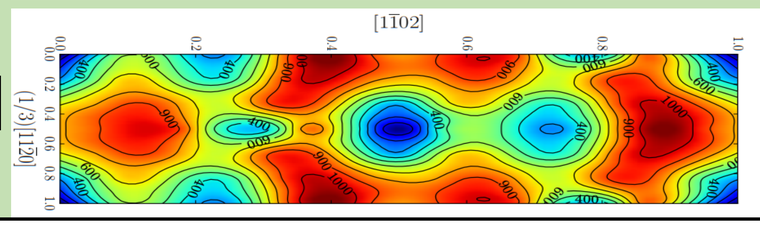
Prismatic Plane

Predicted Splitting:
DFT: 1/3[1-210] → 1/6[1-210] + 1/6[1-210]
TB: 1/3[1-210] → (1/6[1-210] + 0.15[0001]) + (1/6[1-210] - 0.15[0001])

Tight Binding



Pseudopot. [4]



First order Pyramidal Plane.

Predicted Splitting:
Pseudopotential: 1/3[2-1-13] → 4/18[1-102] + 4/18[42-62] + 4/18[2-1-13]
TB: 1/3[2-1-13] → 4/18[1-102] + 4/18[42-62] + 4/18[2-1-13]

Applications:

- ***Alloy design.***
- ***Stress-corrosion cracking.***
- ***Electrochemistry.***

References:

[1] Ghazisaeidi, (2012), *Core structure of a screw dislocation in Ti from density functional theory and classical potentials*
[2] Stassis, D. Arch, B. (1979), *Lattice Dynamics of hcp Ti.*
[3] Rodney, Ventelon (2016), *Ab initio modelling of dislocation core properties in metals and semiconductors*
[4] Ready (2019), *Stacking faults and the γ-surface on {1-101} pyramidal planes in α-titanium.*