Dislocation mediated C migration in Fe Dark Etching Regions

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Motivation

- Rolling contact on bearing raceways generate maximal shear stresses in subsurface.
- Degradation in subsurface microstructure observed due to plasticity.
- This can lead to failure by Rolling Contact Fatigue (RCF).
- Degradation arises in form of Dark Etching Regions (DERs), characterised by development of ferrite features with patches of unaltered martensitic matrix.
- Carbon redistribution is thought to be a fundamental mechanism behind DER formation.
- Dislocation-driven carbon migration has been suggested but hard to experimentally verify.
- Atomistic modelling necessary to ascertain if dislocations move carbon and the underlying mechanism.

Aims

To answer the questions:

- Do dislocations move carbon?
- Do temper carbides dissolve/grow with rolling contact fatigue?

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Objectives

- Build Kinetic Monte-Carlo model of dislocation motion.
- Tight-binding used to obtain formation energies:
    1. Kink-pair formation energies as a function of carbon content and stress.
    2. Dissolution energies of carbon near core of dislocation as a function of stress.

Methods

- Density Functional Theory is not feasible.
- Use tight-binding: rigorous approximation to DFT.
- Boundaries of cell affect relaxation of core more.
- Semi-empirical method is more computationally efficient.

Tight Binding

- Tight binding is an approximation to DFT.
- Overlaps between atomic orbitals are key parameters.
- Parameters can be fitted to experimental data
- $\mathcal{O}(N^3)$, but much smaller prefactor compared to DFT.

BOP

- BOP is a faster but less accurate $\mathcal{O}(N)$ method of interatomic force calculation within tight-binding.
- One builds a local density of states from moments, giving detailed electronic structure information.

Embedding

- Idea is to combine speed of BOP ($\mathcal{O}(N)$) with accuracy of tight-binding $\mathcal{O}(N^3)$.
- Increasing the number of atoms gives freedom to:
  - Investigate isolated dislocations.
  - Include solutes at more realistic concentrations.
  - Simulate interfaces near a surface (e.g. TiO_2 and bulk Ti)

Invariance theorem with green's function approaches. So good with boundary conditions.

Defect Clusters

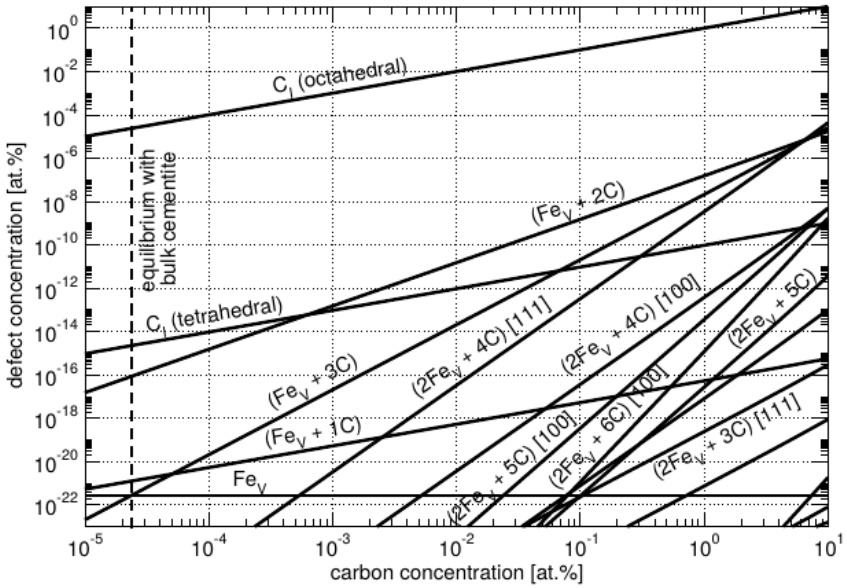
- Increase in oxygen content in Ti-7wt.%Al causes higher number density of α_2 precipitates at 550° C (Felicity's results).
- Oxygen acting as a defactant might stabilise defect complexes (Ti_v + nO).
- This can cause more defects resulting in the increased number of precipitates due to more nucleation sites.
- First starting out with pure Ti and α_2. Still working on extension to Ti-7wt.%Al.

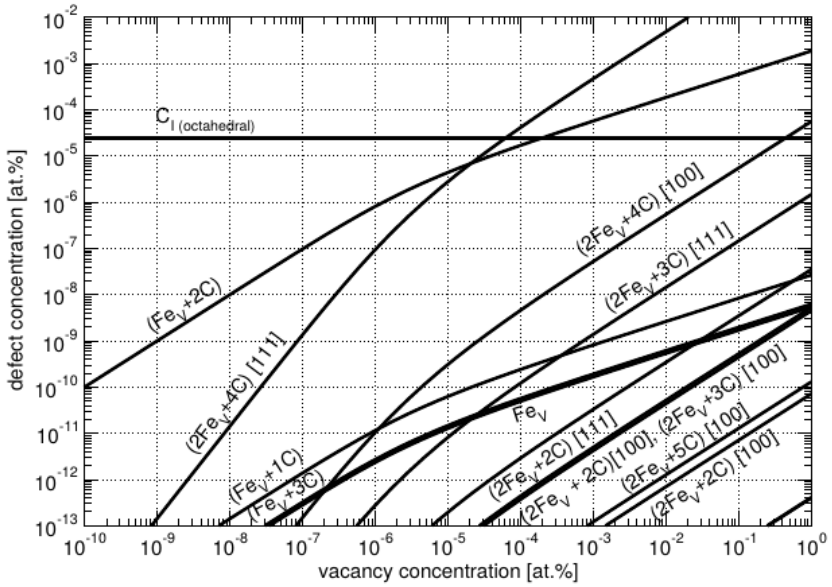
Calculation Details

- Först *et al.* [3] calculated energetics of defect complexes with associated local force-constant matrix.
- Partial thermodynamic equilibrium imposed (thermal equilibrium for one species and not the other).
- Defect concentration plotted as a function of carbon/vacancy concentration only at 160° C.
- Extension: apply the quasiharmonic approximation/do thermodynamic integration for better accuracy at higher temperatures (550° C - 950° C).

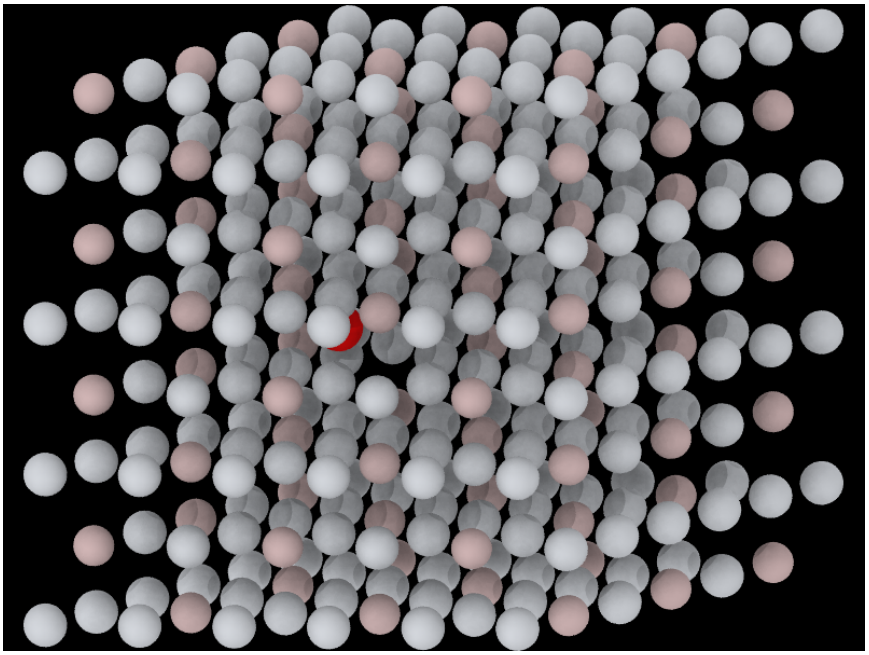
[3] *Point Defect Concentrations in Metastable Fe-C Alloys*, Först *et al*, Phys. Rev. Lett. 96, 2006

Plots in Fe-C


defect concentration [at.%]
carbon concentration [at.%]
equilibrium with bulk cementite
C_I (octahedral)
C_I (tetrahedral)
(Fe_V + 2C)
(Fe_V + 3C)
(Fe_V + 1C)
Fe_V
(2Fe_V + 4C) [111]
(2Fe_V + 4C) [100]
(2Fe_V + 5C)
(2Fe_V + 6C) [100]
(2Fe_V + 5C) [100]
(2Fe_V + 3C) [111]


defect concentration [at.%]
vacancy concentration [at.%]
C_I (octahedral)
(Fe_V+2C)
(2Fe_V+4C) [111]
(Fe_V+1C)
(Fe_V+3C)
(2Fe_V+4C) [100]
(2Fe_V+3C) [111]
Fe_V
(2Fe_V+2C) [111]
(2Fe_V+2C)[100], (2Fe_V+3C) [100]
(2Fe_V+5C) [100]
(2Fe_V+2C) [100]

Ti_3Al Cells



Ti Cells

Defect Clusters: Future Work

- Finish Ti and Ti_3Al defect cluster calculations in DFT.
- Possibly extend to Ti-7wt%Al with SQS structures.
- See how much of an effect anharmonicity has on predictions.

Summary

- Successfully made TB model of Ti which reproduces DFT results with only d-orbitals.
- Transferable:
  - Correct energetic ordering for study of different phases.
  - Correct elastic properties and good scaling for defect simulations.
  - Integer number of electrons for charge transfer models (electrochemistry).

- BOP formulation produces similar results with only linear scaling.
- Embedding calculations should resolve single dislocation core ground-state at realistic O concentrations.
- To do: Embed O-disl, Ti/TiO_2 interface, defect clusters.