Multi-scale investigation of dislocation assisted carbon migration in ferrite

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23.02.2021

Introduction

- Rolling contact on bearing raceways generate maximal shear stresses in subsurface.
- Degradation of subsurface microstructure observed.
- This can lead to failure by Rolling Contact Fatigue (RCF).
- Subsurface degradation arises in form of Dark Etching Regions (DERs).
- DERs characterised by development of ferrite and carbide features with patches of unaltered martensitic matrix.

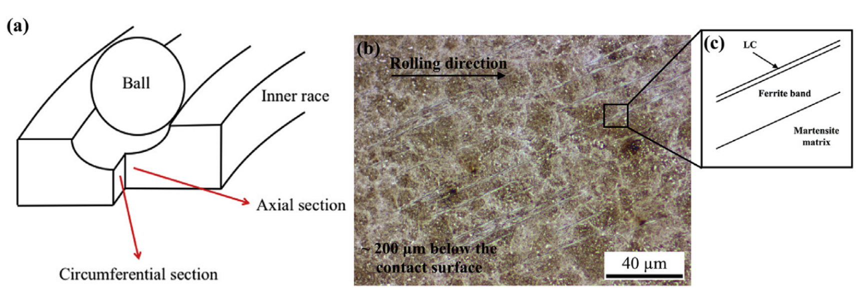

Figure 1: Diagram of DER location within a bearing and its characteristics, [?]

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Motivation

- Carbon redistribution and plastic deformation are thought to be fundamental mechanisms behind DER formation.
- Differing mechanisms of dislocation-driven carbon migration have been suggested, but no consensus.
- Atomistic modelling necessary to elucidate how dislocations could move carbon; thus clarifying potential mechanisms of DER formation.

Aims

To answer the questions:

- How can dislocations assist in carbon migration?
- How are dislocations influenced by carbon on atomistic scale?
  - Is dislocation core structure affected?
  - How does carbon affect kink-pair nucleation/migration?

Methods

- Quantum-mechanical tight-binding simulations used to determine influence of atomistic carbon on dislocations (more accurate than empirical potentials, better scaling than DFT).
- Line tension model of dislocation to acquire stress-dependent kink-pair formation energies.
- Future work is to use kMC model to see what happens at even larger scale of large-scale dislocation movement.

Tight-binding

Cell dislocaton arrangement used to find Peierls potential. Simulation cell used to find binding energies of carbon to screw dislocations.

Peierls Potential

DFT Peierls potential of screw dislocation. Tight-binding Peierls potential of screw dislocation.

Binding of C to screw core

- Distribution of carbon around the easy core dislocation.
- Distribution of carbon around the hard core dislocation.
- The first and second closest octahedral sites to the hard core decay to a prismatic position inside the hard core.

Carbon concentration on dislocation line

- Can solve for the equilibrium carbon concentration on the dislocation line from the Fe-C binding energies around the dislocation core.
- Can include the effect of the C-C first-neighbour repulsive energy, which reduces the overestimation from using the bare McClean Isotherm for the equlilbrium concentration.

$$\{\overline{c_{\mathrm{d}}\mathrm{i}\}\{1-c_{\mathrm{d}}\mathrm{i}\}=\{c\,\mathrm{bulk}\}\{1-c_{\mathrm{bulk}}\}\mathrm{exp}\left(\{E\,\mathrm{b}\,\mathrm{i}\}\{k_{\mathrm{B}}T\}\right)(1)}$$

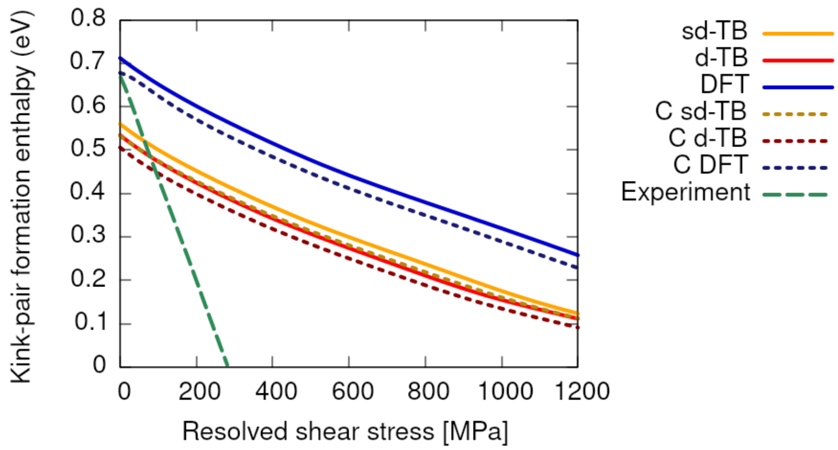
$$N_{\mathrm{oct}}c_{\mathrm{bulk}} + N_d c_d = N_{\mathrm{oct}}c_{\mathrm{nom}}/3 \tag{2}$$

Line tension

$$E_{\mathrm{LT}} = \frac{K}{2}\sum_j(\vec{P}_j-\vec{P}_{j+1})^2+\sum_j \Delta E_{\mathrm{P}}(\vec{P}_j)+(\sigma\cdot\vec{b})\times\vec{l}\cdot\vec{P}_j-\sum_{j,k}E_{\mathrm{C}}(|\vec{P}_j-\vec{P}^{\mathrm{C}}_k|),$$

- Equation used for the line tension model.
- The interaction between solutes is parameterised with a lorentzian.

Kink-pair formation enthalpies



- The addition of carbon reduces the kink-pair formation enthalpy.
- The reduction is less than one would expect from hydrodgen as the interaction with carbon is longer ranged due to the large tetragonal distortion and binding energies.

Summary

- Obtained Peierls potential and binding energies of carbon distributed around hard and easy screw dislocation cores from quantum-mechanical atomistic simulations.
- Calculated the equilibrium concentration of carbon on the dislocation line by calculation of C-C repulsive energies.
- Find that **all** dislocations are hard core, at typical dislocation densities, nominal carbon concentrations and temperatures, due to the reconstruction of easy core due to carbon-dislocation interaction and operating temperatures.
- Carbon decreases the stress necessary to move the screw dislocations at all temperatures.