Multi-scale investigation of dislocation mediated carbon migration in iron

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Contents

Abstract

We investigate the validity of a dislocation-assisted carbon migration mechanism underpinning the formation of dark etching regions in bearing steels undergoing high-cycle fatigue through use of a multi-scale approach: from quantum mechanics, to stochastic simulations. We start from tight binding simulations of $1/3\langle 111\rangle$ screw dislocations to obtain the 2-d Peierls potential and Fe-C binding energies. These become ingredients for a line-tension model of the $1/3\langle 111\rangle$ screw dislocation to obtain the kink-pair formation energy as a function of stress and carbon concentration. Finally, 3-d kinetic Monte-Carlo simulations of dislocations in an environment of carbon are used to ascertain which temperature and stress regimes dislocation-assisted carbon migration is a valid mechanism.

Introduction

Computational Method

- Use tight-binding model of Paxton and Elsaetter (0,).
- Generate dislocations using anisotropic elasticity theory.
- Create clusters of dislocations in both easy and hard core configurations.
- Place carbon in octahedral sites around the core
- Calculate corrections (ZPE etc)

Results

Peierls Potential

To determine the Peierls potential, we followed the procedure detailed in Itakura (0,). Quadrupolar arrays of dislocations were constructed by placing dislocations of antiparallel $1/2\langle 111\rangle$ Burgers vectors in an "S" arrangement (0,), with initial displacements determined by the anisotropic elasticity solutions. These displacements were modified to be periodic, thereby removing artificial stacking faults which would appear between periodic images after the introduction of the dipole. This was achieved by the subraction of a linear error term from the superposition of displacement fields arising from the dislocations in the simulation cell and its periodic images (0,). To accomodate for the internal stress upon introduction of the dislocation dipole into a simulation cell, an elastic strain was imposed on the cell, resulting in an extra tilt component being added to the cell vectors (0, ,). Simulation cells were constructed with different initial core positions, which were sampled from the triangular region "EHS" (easy, hard and split) core positions, as detailed in 1. To fix the dislocation positions during relaxation, the three atoms surrounding the easy core, for each dislocation, were fixed during relaxation.

Comparison of 2d Peierls potentials of the $1/2\langle 111\rangle$ screw dislocation between DFT can by found in (0,). Data was interpolated using 2d cubic splines. "E", "H" and "S" correspond to easy, hard and split core positions respectively, with the latter also corresponding to atomic positions. The relative energies between the different core positions is smaller in tight-binding compared to DFT; most notably, the energies. This is an artifact in the model, which has been validated in NEB calculations of the $1/2\langle 111\rangle$ screw dislocation Peierls barrier, as calculated with NEB, is roughly half that when compared to DFT **INSERT LUKES THESIS REFERENCE**. The split core as seen in tight-binding is reminiscent of EAM potentials, where the split core energy is lower than that of the hard core.

This may be attributed to lack of core electron repulsion, resulting from the sd-iron tight-binding model.

Hard and easy core relaxations

To determine the binding energy of carbon, we first relaxed clusters of atoms, with $R_1 = $ simulation cells of each core in the cluster method. The three atoms surrounding the core were

As found in DFT simulations by Ventelon (0,), when a carbon was placed in the vicinity of a relaxed easy dislocation core—in either of the two nearest, distinguishable, oc-

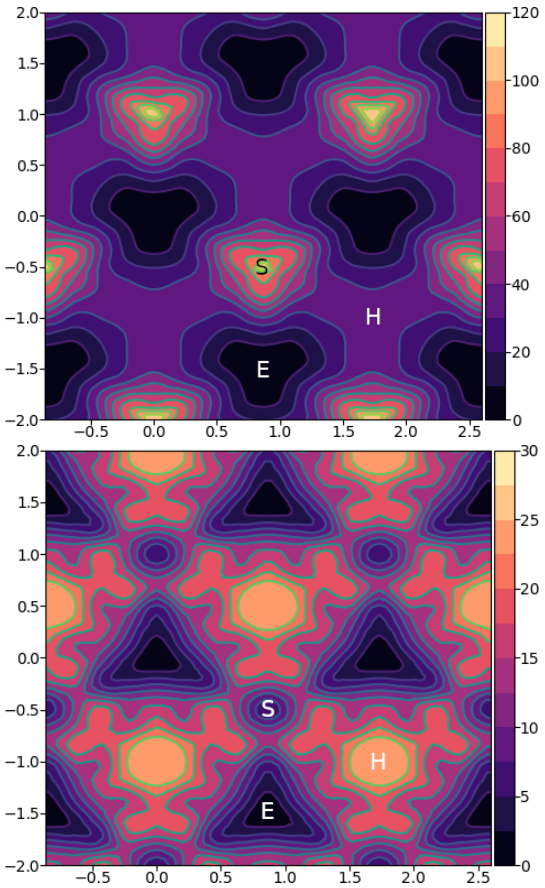


Table 1

Comparison of 2d Peierls potentials of the $1/2\langle 111\rangle$ *screw dislocation between DFT cite:Itakura2012 (top) and tight-binding (bottom). Data was interpolated using cubic splines. Energies are in meV, with x and y scales in units of* $\sqrt{2}a_{bcc} = 2\sqrt{2/3}b$*. "E", "H" and "S" correspond to easy, hard and split core positions respectively, with the latter also corresponting to atomic positions. The relative energies between the different core positions is smaller in tight-binding compared to DFT. The split core as seen in tight-binding is reminiscent of EAM potentials, where the split core energy is lower than that of the hard core. Some of this discrepancy can be attributed to the difference in simulation method: the cluster method may inhibit the relaxation of the core more than quadrupolar cells, due to finite size effects.*

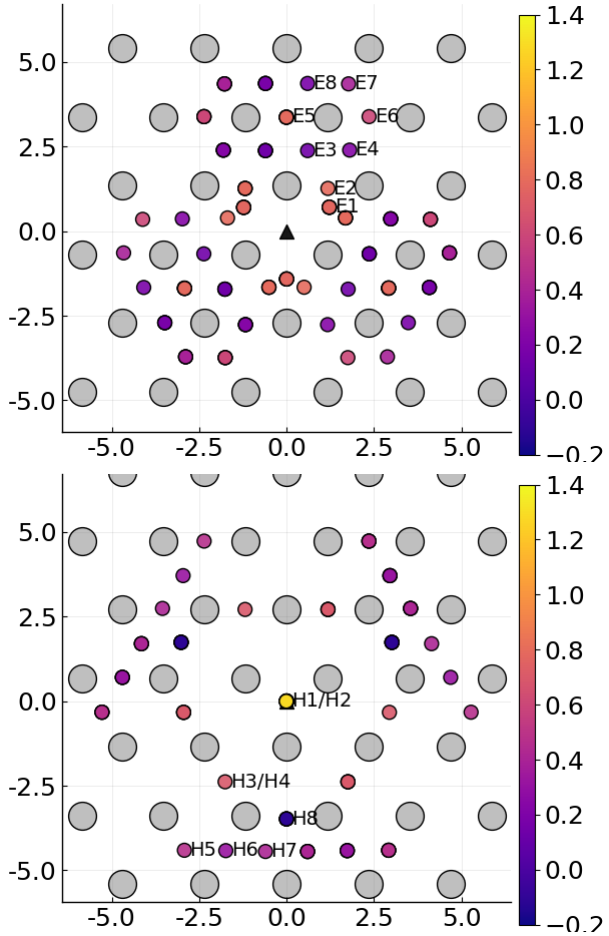
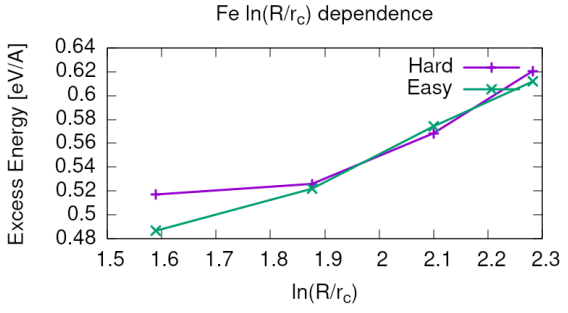


Table 2

Final positions and binding energies (eV) of carbon around the the easy core (top) and hard core (bottom). The core was constrained by fixing the top and bottom three atoms surrounding each of the cores. As shown by Ventelon cite:Ventelon2015, the first and second closest octahedral sites to the hard core have their minimum energy inside the hard core.

tahedral sites—a spontaneous reconstruction of the dislocation core occurred: from easy to hard. Upon reconstruction, the dislocation core moved to a neighbouring triangle, when looking along the $\langle 111\rangle$ direction, where the carbon found itself situated in the centre.



Plot of dislocation energy as function of cluster size.

Following the paper by Itakura (0,) we calculated the binding energy of carbon each of the screw dislocation cores.

The solution energy is given by

$$E_s = E_{\mathrm{d+C}} - E_{\mathrm{d}} - E_{\mathrm{C\,oct.}},$$

where $E_{\mathrm{d+C}}$ is the total energy of a relaxed cluster with a carbon interstitial and a dislocation, E_{d} is the total energy of a relaxed cluster with a dislocation and $E_{\mathrm{C\,oct.}}$ is the total energy of relaxed a cluster with a single carbon in an octahedral site.

The zero-point energy is calculated as in Itakura. A 3x3 Hessian matrix is constructed by taking the numerical derivative of the forces observed on the carbon atom after displacement by ±0.015Å in each of the X, Y and Z directions. The zero-point energy is given by

$$E_z = \frac{1}{2}\sum_{i=1}^{3}\frac{h}{2\pi}\sqrt{k_i/m_{\mathrm{C}}},$$

where k_i are the eigenvalues of the Hessian and m_{C} is the mass of carbon.

The ZPE corrected solution energy is given by

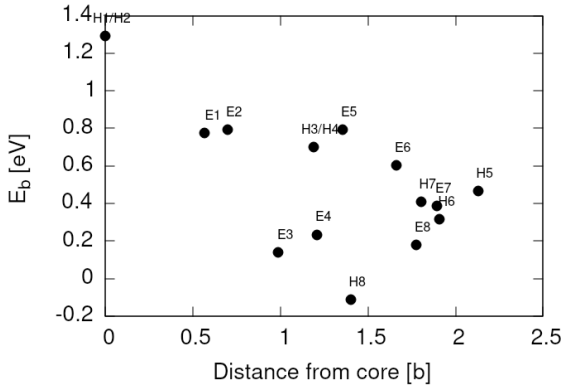
$$E_s^{\mathrm{Z}} = E_s + E_z - E_{z\mathrm{C\,oct.}},$$

v where $E_{z\mathrm{C\,oct.}} = 202.5meV$ is the zero-point energy of carbon situated in an octahedral site in a perfect cluster of the same size.

Table of relaxed

Site Type	E_b^z eV	distance from core [b]	distance from core Å
E1	0.775	0.57	1.413699
E2	0.793	0.70	1.732527
E3	0.139	0.99	2.458179
E4	0.234	1.21	3.001665
E5	0.791	1.36	3.369997
E6	0.603	1.66	4.129084
E7	0.388	1.89	4.703422
E8	0.178	1.77	4.409563
H1/H2	1.291	0.00	0.000472
H3/H4	0.698	1.19	2.960187
H5	0.467	2.12	5.287079
H6	0.316	1.91	4.746490
H7	0.409	1.80	4.483550
H8	-0.114	1.40	3.480325

These binding energies agree well with experiment and previous calculations. The maximum binding energy found by



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