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 (Paxton & Elsässer, 2013).
- 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

Dislocation core energy landscapes

Hard and easy core relaxations

Plot of dislocation energy as function of cluster size.

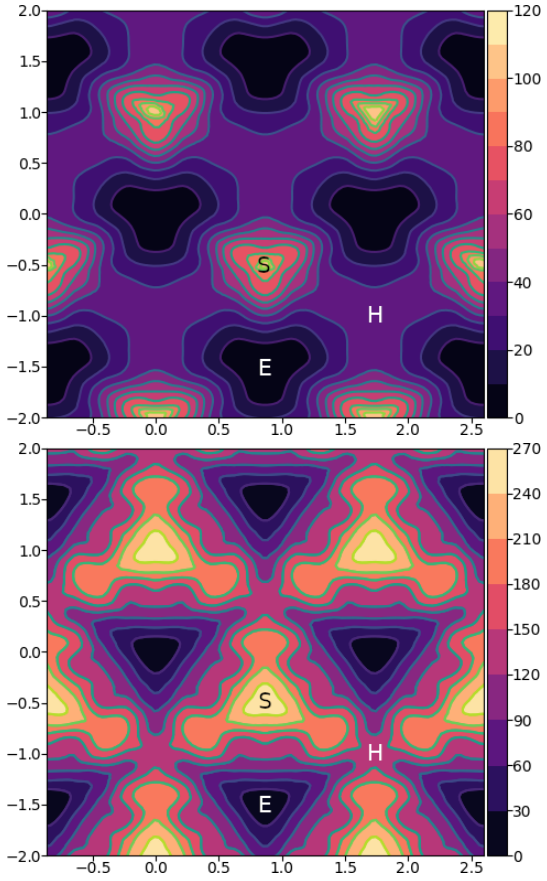


Table 1
Comparison of 2d Peierls potentials of the $1/2\langle 111\rangle$ *screw dislocation between DFT cite:Itakura2012 (top) and tight-binding (bottom). Data was interpolated using cubic splines. Energies are in meV, with x and y scales in units of* $\sqrt{2}a_{bcc} = 2\sqrt{2/3}b$. *"E", "H" and "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 larger in tight-binding compared to DFT. 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.*

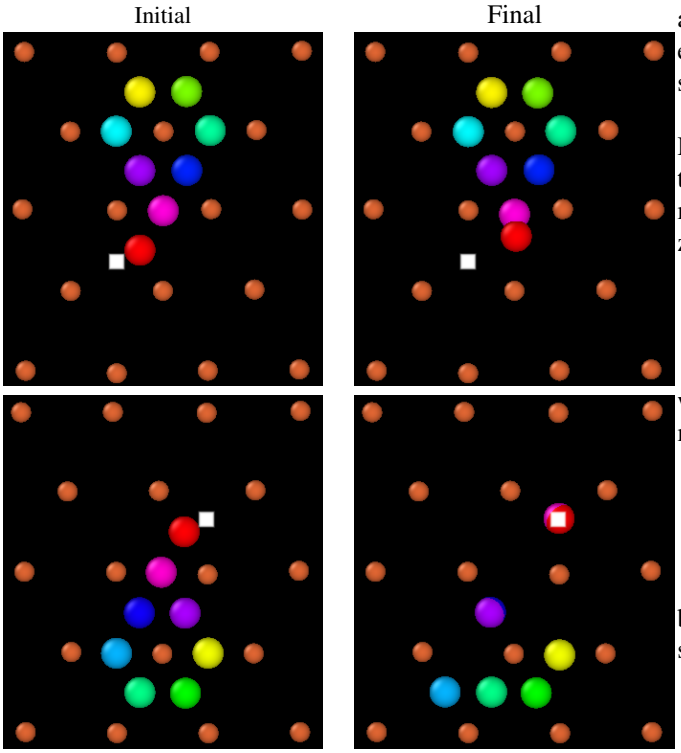
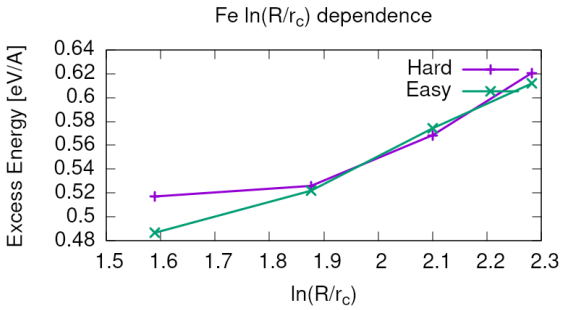


Table 2
Initial and final octahedral sites for the easy core (first row) and the hard core (second row). As shown by Ventelon cite:Ventelon2015, the first and second closest octahedral sites to the hard core have their minimum energy inside the hard core, but we do not find that the easy core reconstructs into a hard core, with these same sites.



Following the paper by Itakura (Itakura, Kaburaki, Yamaguchi, & Okita, 2013) 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

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

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 energies.

Site Type	$E_{\mathrm{d+C}} - E_{\mathrm{d}}$)	E_s	$E_z - E_{z\,\mathrm{C\,oct.}}\ meV$	E_z^b r
E1	-0.89299636	-0.05828365	-17.8194	-775
E2	-0.89300553	-0.05829282	-0.529601	-792.
E3	-0.84476459	-0.01005188	2.47361	-139.
E4	-0.85151735	-0.01680464	5.36252	-234.
E5	-0.89232261	-0.0576099	7.63124	-791.
E6	-0.87856485	-0.04385214	6.60286	-603.
E7	-0.86299687	-0.02828416	3.21964	-388.
E8	-0.84773572	-0.01302301	0.35220	-177.
H1/H2	-0.93009177	-0.09537906	-6.39993	-129
H3/H4	-0.88549598	-0.05078327	7.3888	-698.
H5	-0.86857644	-0.03386373	6.5459	-467.
H6	-0.85757695	-0.02286424	4.6842	-315.
H7	-0.8643446	-0.02963189	6.1659	-409.
H8	-0.82596378	8.74893 (-3)	4.7335	114.

Distance dependence of binding energies.

Bibliography

References

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