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

Hard and easy core relaxations

Plot of dislocation energy as function of cluster size.

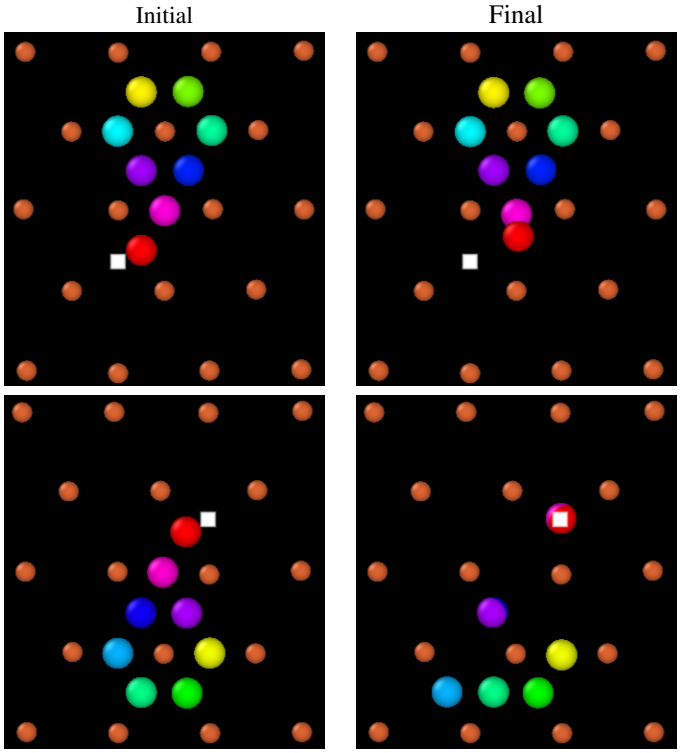
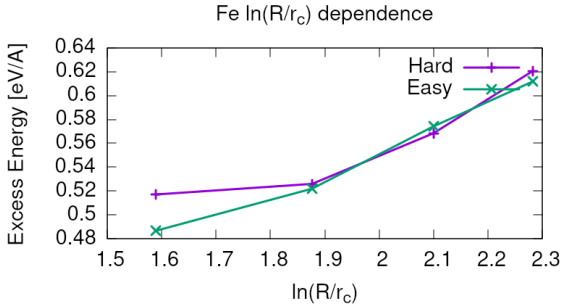


Table 1
Initial and final octahedral sites for the easy core (first row) and the hard core (second row). As shown by Ventelon cite:Ventelon2015, the first and second closest octahedral sites to the hard core have their minimum energy inside the hard core, but we do not find that the easy core reconstructs 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.

Distance dependence of binding energies.

Site Type	$E_{\mathrm{d+C}} - E_{\mathrm{d}})$	E_s	$E_z - E_{z\,\mathrm{C\ oct.}}\ meV$	$E_z^b\ meV$	distance from core
E1	-0.89299636	-0.05828365	-17.8194	-775.17	1.413699
E2	-0.89300553	-0.05829282	-0.529601	-792.585	1.732527
E3	-0.84476459	-0.01005188	2.47361	-139.236	2.458179
E4	-0.85151735	-0.01680464	5.36252	-234.001	3.001665
E5	-0.89232261	-0.0576099	7.63124	-791.454	3.369997
E6	-0.87856485	-0.04385214	6.60286	-603.242	4.129084
E7	-0.86299687	-0.02828416	3.21964	-388.045	4.703422
E8	-0.84773572	-0.01302301	0.35220	-177.539	4.409563
H1/H2	-0.93009177	-0.09537906	-6.39993	-1291.2	0.006472
H3/H4	-0.88549598	-0.05078327	7.3888	-698.231	2.960187
H5	-0.86857644	-0.03386373	6.5459	-467.286	5.287079
H6	-0.85757695	-0.02286424	4.6842	-315.768	4.746490
H7	-0.8643446	-0.02963189	6.1659	-409.228	4.483550
H8	-0.82596378	8.74893 (-3)	4.7335	114.302	3.480325

Bibliography

References

Itakura, M., Kaburaki, H., Yamaguchi, M., & Okita, T. (2013). The effect of hydrogen atoms on the screw dislocation mobility in bcc iron: a first-principles study. *Acta Materialia*, *61*(18), 6857-6867. Retrieved from https://doi.org/10.1016/j.actamat.2013.07.064 doi: 10.1016/j.actamat.2013.07.064

Paxton, A. T., & Elsässer, C. (2013, June). Analysis of a carbon dimer bound to a vacancy in iron using density functional theory and a tight binding model. *Physical Review B*, *87*(22). Retrieved from https://doi.org/10.1103/physrevb.87.224110 doi: 10.1103/physrevb.87.224110