

Multi-scale investigation of dislocation mediated carbon migration in iron

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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.

1 Introduction

Martensitic steels are frequently used in bearings due to their resilience to service conditions, being subject to high rotational speeds and contact pressures. However, under cyclic loading exceeding a given contact stress, the microstructure of the steel can decay due to the accumulation of plasticity. This signals the onset of rolling cycle fatigue (RCF), which increases the risk of failure from subsurface crack initiation. The microstructural decay corresponds to the observation of Dark Etching Regions (DERs) as seen in optical microscopy, where the darkness of these regions is due to the higher reactivity of the phases which compose the DER to the etchant; exacerbated by the roughness of the DER region.

Carbon within the martensitic matrix at normal operating temperatures has a low diffusivity; as such it cannot segregate out of the martensite. A plausible mechanism for the degradation of the martensitic microstructure is a process of carbon migration, driven by dislocation glide, described as follows [CITATION]. Due to the high dislocation density exhibited in martensite, carbon segregates to dislocations in Cottrell atmospheres, causing pinning. Strain generated by cyclic stresses allow dislocations to escape their carbon rich environment. The dislocations, now free, re-attract carbon, allowing the Cottrell atmosphere to reform, subsequently re-pinning the dislocations, creating a net carbon flux.

structure of a WEB consisting of a ferrite band and a LC adjacent to it. One can see the DER region is composed of regions of ferrite interspersed in the parent martensite with lenticular carbides bordering the ferrite bands.

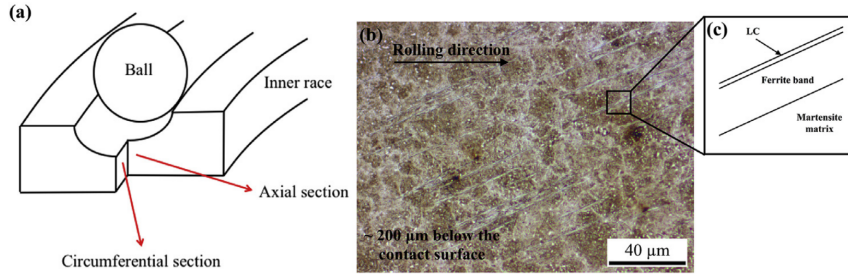


Figure 1: Diagram of where DER occurs and its characteristics, taken from [1]. (a) Axial and Circumferential sections of a bearing inner ring. (b) Circumferential section of a bearing inner ring under optical microscope, where ferrite bands (white etching bands) are formed at the subsurface with an inclination angle of 30° to the rolling direction. (c) Diagram showing the

Through dislocation-assisted carbon migration, martensite transforms to ferrite (microband and elongated forms). Residual carbides, untouched at the start of DER formation, gradually dissolve as a result of highly localised

plasticity: dislocation rearrangement and pile ups at the interface draw carbon atoms out. Further RCF progression leads to the formation of low and high angle ferrite features, White Etching Bands (WEBs), composed from the microband and elongated ferrite. Carbon migration through dislocation motion allows carbon to move from the martensitic matrix—and (partially) dissolved residual carbides—to form lenticular carbides between these ferrite bands.

However, fundamentals behind DER formation through this process remain contentious. It is not definitively known where carbon migrates to with the onset of DER formation: where does excess carbon from the martensitic matrix find itself, when the structure decays to low solubility (0.02%) ferrite? It is not known whether carbon atoms inside the martensite are transported towards the residual transition carbides, [2], or if they segregate to the boundaries of ferrite microbands/elongated ferrite.

Fu *et al.* propose that carbon atoms inside the martensite would segregate to pre-existing/residual carbides, increasing their size [2]. This theory has been successfully applied to the growth of lenticular carbides [1], however, problems arise with their application to the growth of residual carbides: if carbides were to form in martensite, they should follow the Bagaryatskii/Isaichev orientation relationship, but observations suggest a lack of any orientation relationship [3]. Carbides formed within the DER region have an irregular shape/diffuse boundaries, which are seemingly due to the incomplete *dissolution* of *residual* carbides, which is at odds with the theory of Fu *et al.* and residual carbide growth.

Probing the fundamental mechanisms behind DER formation experimentally have proven difficult and inconclusive. Work needs to be done to understand dislocation-carbon interactions, more specifically, how dislocations can move carbon within the temperature and stress regimes experienced during operation, and what phenomena occur during dislocation-assisted carbon migration. This is vital to understanding martensite decay and DER formation. With further knowledge of the fundamental mechanism behind DER formation, we can suppress dislocation motion in the martensitic matrix, mitigating failure by RCF.

To shed light on the fundamental mechanism underpinning DER formation—dislocation-assisted carbon migration—a multi-scale modelling approach can be used. Atomistics can provide information of the 2d Peierls energy landscape which dislocations are subject to in iron; and how this landscape is modified by the binding of carbon to dislocations. This data can be used in a line tension model of a dislocation, to determine the kink-pair nucleation energies of dislocations as a function of carbon content and stress. Finally, one can use a kinetic Monte Carlo model of dislocation glide, by thermally activated kink-pair nucleation, in an environment of carbon. From this last stage of coarse-graining, one can determine in which regimes of temperature, stress and carbon concentration, dislocation-assisted carbon migration becomes a

feasible mechanism behind DER formation, with predictions of dislocation velocity and where carbon moves to as dislocations glide. In this report, we will focus on the atomistic portion of this project, directed at understanding dislocation-carbon interactions at the atomistic scale in bcc iron, which will feed into the line-tension model of dislocation kink-pair formation.

2 Computational Method

We use the tight-binding model of Paxton and Elsätter [4], which has been shown to describe the binding energies of carbon complexes in bcc iron, in good agreement with high-quality Density Functional Theory (DFT) calculations. This model reproduces the two screw dislocation core structures—the easy and hard $1/2\langle 111 \rangle$ cores—exhibited in bcc iron, which are crucial to understanding solute-dislocation interactions in bcc iron. Hydrogen and carbon have been shown to reconstruct these cores into the, usually metastable, hard core from the easy core [5, 6]. Computationally cheaper models, which do not incorporate quantum mechanics, such as the EAM, cannot reproduce these behaviours.

To determine the Peierls potential of a $1/2\langle 111 \rangle$ screw dislocation, we followed the procedure detailed in Itakura [7]. Quadrupolar arrays of dislocations were constructed by placing dislocations of antiparallel $1/2\langle 111 \rangle$ Burgers vectors in an "S" arrangement [8], see ??, 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 dislocation dipole. This was achieved by the subtraction of a linear error term from the superposition of displacement fields arising from the dislocations in the simulation cell and its periodic images [9]. To accommodate for the internal stress upon introduction of the dislocation dipole into a simulation cell, an elastic strain was applied to the cell, resulting in an additional tilt component added to the cell vectors [8, 9]. 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 ?. To fix the dislocation positions during relaxation, the three atoms surrounding the easy core, for each dislocation, were fixed in Z coordinate during relaxation. Relaxations were carried out until forces on each atom were less than $1 \times 10^{-3} \text{eV}^{-1}$.

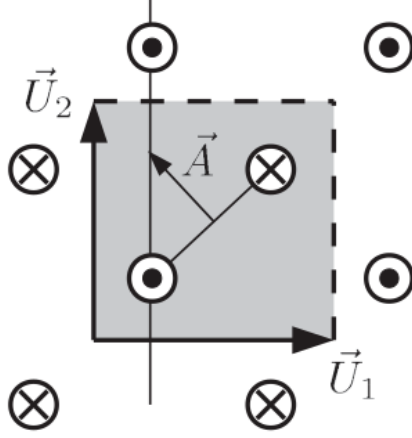


Figure 2: Figure of the quadrupolar arrangement used to determine the Peierls potential. \vec{U}_1 and \vec{U}_2 are the periodicity vectors in the X-Y plane. \vec{A} is the vector defining the cut plane of the dislocation dipole [8].

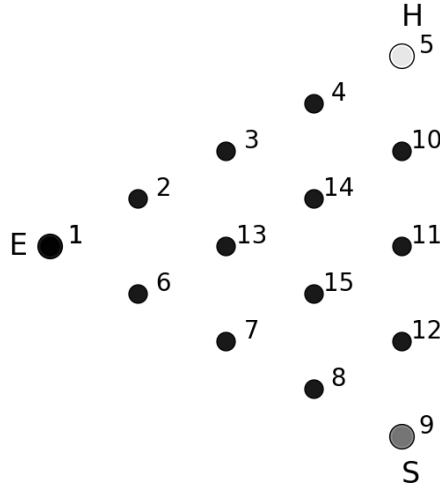


Figure 3: Figure of the sampled positions used to determine the the Peierls potential. "E", "H" and "S" correspond to the easy, hard and split core positions respectively.

The interaction energy between the dislocation dipole and periodic images was defined differently to that of Itakura's. We followed the prescription of Bulatov and Cai [9] to find a regularised interaction energy, which is independent of truncation limit, in contrast to the formulas quoted in Itakura's papers [7]. Details can be found in 7.1.

The Peierls potential here is defined relative to the energy of the easy core configuration. The difference in total energies is taken between a relaxed cell, where the dislocation cores are displaced, from the periodic easy core

reference, with a correction term coming from the difference in interaction energies between the displaced state and the easy core, due to the difference in dislocation positions. Δ henceforth refers to quantities relative to the easy core configuration, divided by the total number of dislocations in the reference cell.

$$\Delta E_P = \Delta E^{\text{tbe}} - \Delta E_{\text{INT}}$$

To determine the binding energy of carbon to dislocations, we used the cluster method: simulation cells consist of a cylindrical cluster of atoms, with a single dislocation introduced into the centre using displacements from the anisotropic elasticity solutions. Each of the clusters were centred on the easy or hard core positions. The cluster of atoms was split into two regions: a central region of dynamic atoms with radius R_1 , and an annulus of atoms, between R_1 and R_2 , which were fixed to the anisotropic elasticity solutions.

Initially, large cells of with $R_1 = 6\sqrt{2}a_{\text{bcc}}$, and $R_2 = 7\sqrt{2}a_{\text{bcc}}$ and depth of single burger's vector, were relaxed for both the easy and hard cores, which consisted of 522 and 540 atoms respectively. The three atoms surrounding the core were constrained, to only relax in $X-Y$ plane, to stop the core from moving upon relaxation. The k-point sampling mesh for each of these cells was $1 \times 1 \times 24$, with a charge tolerance for self-consistency of 1×10^{-6} . Atoms were relaxed until the force on each atom was less than $1 \times 10^{-3} \text{ eV\AA}^{-1}$.

From the relaxed cells, a smaller region of 174 atoms, with $R_1 = 3\sqrt{2}a_{\text{bcc}}$, and $R_2 = 4\sqrt{2}a_{\text{bcc}}$, was cut from the dynamic regions. This smaller cell was extended to a thickness of $3b$ in the Z direction. Carbon interstitials were inserted into octahedral sites near the dislocation core, in the middle layer. Exploiting reflection and rotational symmetry, allows us to use only 10 interstitial sites to obtain the binding energies of carbon $\sim 2b$ from the core.

The three atoms surrounding the core in the first and third layers were again constrained to relax only in the X and Y directions. No such constraints were imposed on the middle layer.

Following the paper by Itakura [6] we calculated the binding energy of carbon each of the screw dislocation cores.

The solution energy is given by

$$E_s = E_{\text{d} + \text{C}} + E_{\text{Perfect}} - E_{\text{d}} - E_{\text{C ref.}},$$

where $E_{\text{d} + \text{C}}$ 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 $E_{\text{C oct.}}$ 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. After relaxation of the C-dislocation system, a 3×3 Hessian matrix is constructed by taking the numerical derivative of forces observed on the carbon atom after displacement

by ± 0.015 in each of the X , Y and Z directions. The three atoms surrounding the core on the first and third layers were again fixed in Z coordinate. The zero-point energy is given by

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

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

$$E_s^Z = E_s + \Delta E_z,$$

where $\Delta E_z = E_z - E_{zC \text{ ref.}}$ and $E_{zC \text{ ref.}} = 202.5 \text{ meV}$ is the zero-point energy of carbon situated in an octahedral site in a perfect cluster of the same size. The difference in zero-point energy was found to be negligible in comparison to the binding energies, as one would expect from an atom much larger than hydrogen.

3 Results

3.1 Peierls Potential

Comparison of 2d Peierls potentials of the $1/2\langle 111 \rangle$ screw dislocation between DFT and tight-binding can be found in 1. 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: the tight-binding Peierls barrier half that of DFT [10]. 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 [7]. Some of this discrepancy can be attributed to the erroneous interaction term included by Itakura, as detailed above—interaction energies can become arbitrarily high, if not made independent of truncation limit—but likely, there are effects in DFT which are not encapsulated fully within tight-binding (or EAM), such as a lack of core electron repulsion or environmental dependence.

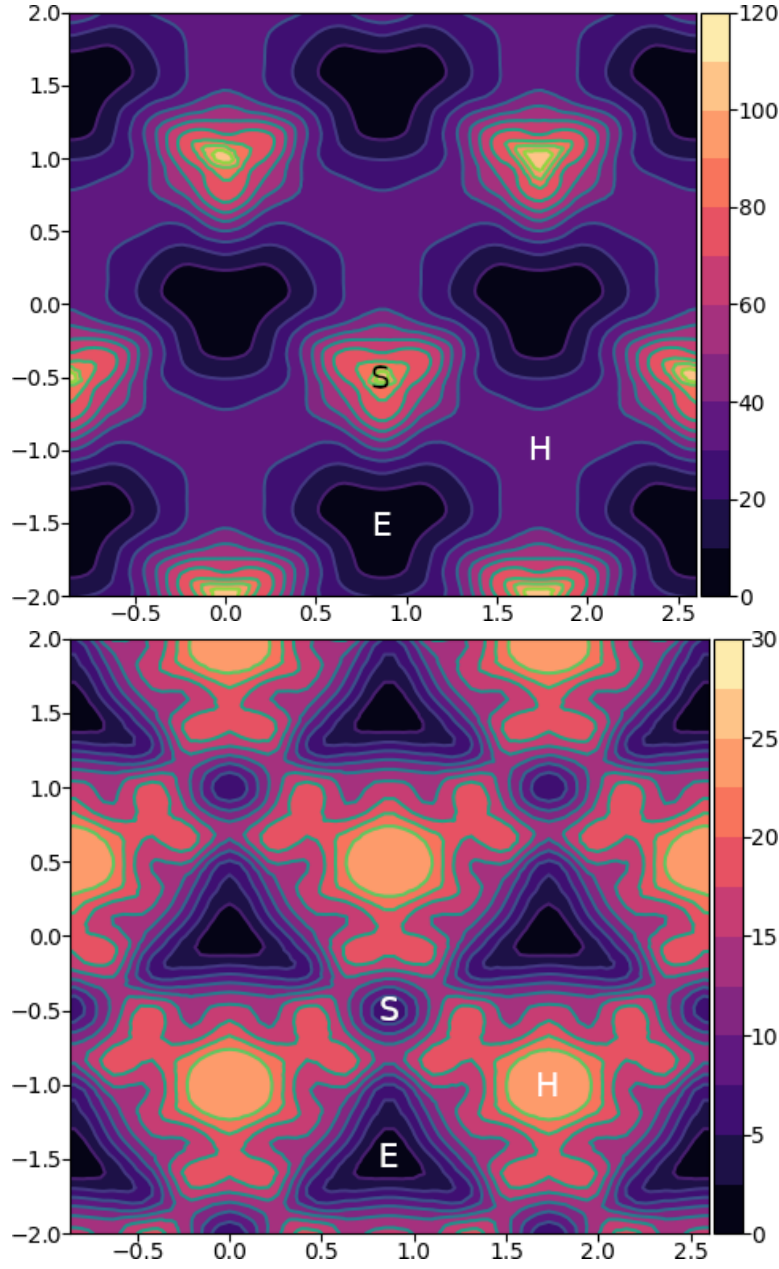


Table 1: Comparison of 2d Peierls potentials of the $1/2\langle 111 \rangle$ screw dislocation between DFT cite:Itakura2012 (top) and tight-binding (bottom). Data was interpolated using cubic splines. Energies are in meV , with x and y scales in units of $\sqrt{2}a_{bcc} = 2\sqrt{2/3}b$. "E", "H" and "S" correspond to easy, hard and split core positions respectively, with the latter also corresponding 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 interaction energy definitions.

Pos	ΔE_{INT}	ΔE_{tbe}	ΔE_{P}	$\Delta E_{\text{P}}^{\text{DFT}}$
1	0	0	0	0
2	-0.7	7.3	7.9	3.2
3	-1.4	16.0	17.4	19.2
4	-2.0	22.2	24.2	31.1
5	-2.5	24.8	27.4	39.3
6	-3.3	3.0	6.3	11.5
7	-6.5	7.1	13.6	39.9
8	-9.6	13.0	22.6	75.2
9	-12.5	5.4	17.9	108.9
10	-4.8	22.1	26.9	34.8
11	-7.2	18.2	25.4	37.9
12	-9.8	14.0	23.8	60.7
13	-3.8	11.5	15.3	17.6
14	-6.9	15.1	22.0	29.9
15	-4.3	18.6	22.9	39.7

3.2 Hard and easy core relaxations

To validate the cluster simulation method, the excess energy, defined as the difference in energy between a cell with a dislocation, and a perfect reference cell, was plotted as a function of $\ln(R/r_c)$, where $R = R_2$ of the cluster and $r_c = b$, is the core radius, as seen in figure ???. In elasticity theory, this should give a linear dependence where the gradient corresponds to combinations of elastic constants. This is well reproduced by our model, except at low $\ln(R/r_c)$ as expected, where the cell size is not large enough to accommodate for sufficient relaxation of the dislocation cores. This increases the core energy, which elasticity theory does not account for.

As found in DFT simulations by Ventelon [5], when a carbon was placed in the vicinity of a relaxed easy dislocation core—in either of the two nearest, distinguishable, octahedral 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. This will be called a prismatic site, as in Ventelon’s paper. This model successfully reproduces this behaviour, confirming that both hard and easy dislocation cores must be studied to fully understand screw dislocation behaviour in bcc iron.

The core energy difference can be estimated by the difference between of excess energies between the easy and hard cores in the limit that $\ln(\frac{R}{R_0}) \rightarrow 0$. At the smallest value, one finds that the core energy difference $\Delta E_c^{\text{Easy-Hard}} = 76 \text{ meV/b}$. This is in agreement with the results of Itakura [7], of 82 meV/b .

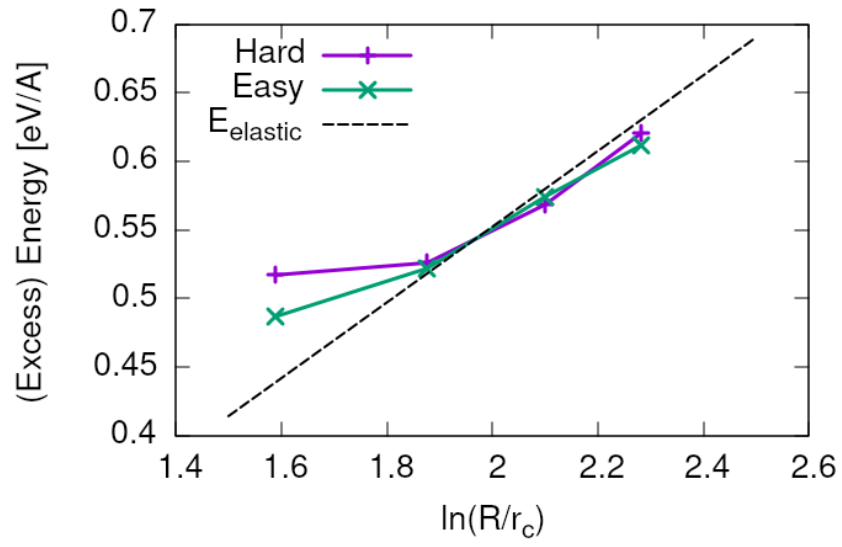


Figure 4: Excess energy of dislocation clusters with differing radii for both the easy and hard core configurations. The prediction from elasticity theory is given by the black, dashed line. Deviation of both cores occur when cell size is small, creating an increase in the core energy, which elasticity theory cannot account for.

3.3 Fe-C binding energies

The binding energies, and distribution, of carbon to both the hard and easy cores can be seen in table 5 and figures 3 and 4. The distribution of carbon strongly depends on the type of core it finds itself situated near.

The easy core only significantly modifies the position of the iE1 site, to the E1 site, situated in the centre of an adjacent triangle. All other sites are unaffected, so there is a one-to-one correspondence between all iEx and Ex sites. There are carbon basins available close to the core, but not inside: a pseudo-prismatic site is not favourable.

Carbon favours a prismatic site within the hard core (H1), which has the highest binding energy of all sites in both cores of 1.29 eV. There are no binding sites apparent in a triangular annulus (of width $\sqrt{2}/2a_{\text{bcc}}$) surrounding the hard core triangle due to the destruction/volume reduction of octahedral sites near the hard core. The initial "octahedral" sites, iH1 and iH2 decay to the H1 site. Similarly, iH3 and iH4 decay to the H2 site, with iH9 and iH10 decaying to a H7 site. Relations between each of the sites is given in table ??.

Table 2: Decay relations between the initial and final sites upon relaxation of carbon interstitials around the hard core.

Initial	Final
iH1, iH2	H1
iH3, iH4	H2
iH5	H3
iH6	H4
iH7	H5
iH8	H6
iH9, iH10	H7

Note that interactions between carbon atoms around the core are not taken into account here: figures 3 and 4 are purely diagrammatic and not what one expects the true distribution of carbon would be around a screw dislocation. Carbon is strongly repulsive at first nearest-neighbour distances, which would modify each of these distributions. Further work is necessary to elucidate the equilibrium distribution at different carbon concentrations.

These binding energies agree well with experiment and previous calculations. Kamber *et al.* found a maximum binding energy of 0.5 eV. Cocharadt found a value of 0.71 eV, which is within 0.1eV of the largest binding energy for the easy core.

EAM calculations by Clouet [11, 12] found a maximum binding energy of 0.41 eV by calculating the elastic dipole tensor within Eshelby theory. Hanlumuayang *et al.* [13], similarly conducted DFT and EAM calculations for the interaction energy 12Å from the core, and their calculations agreed

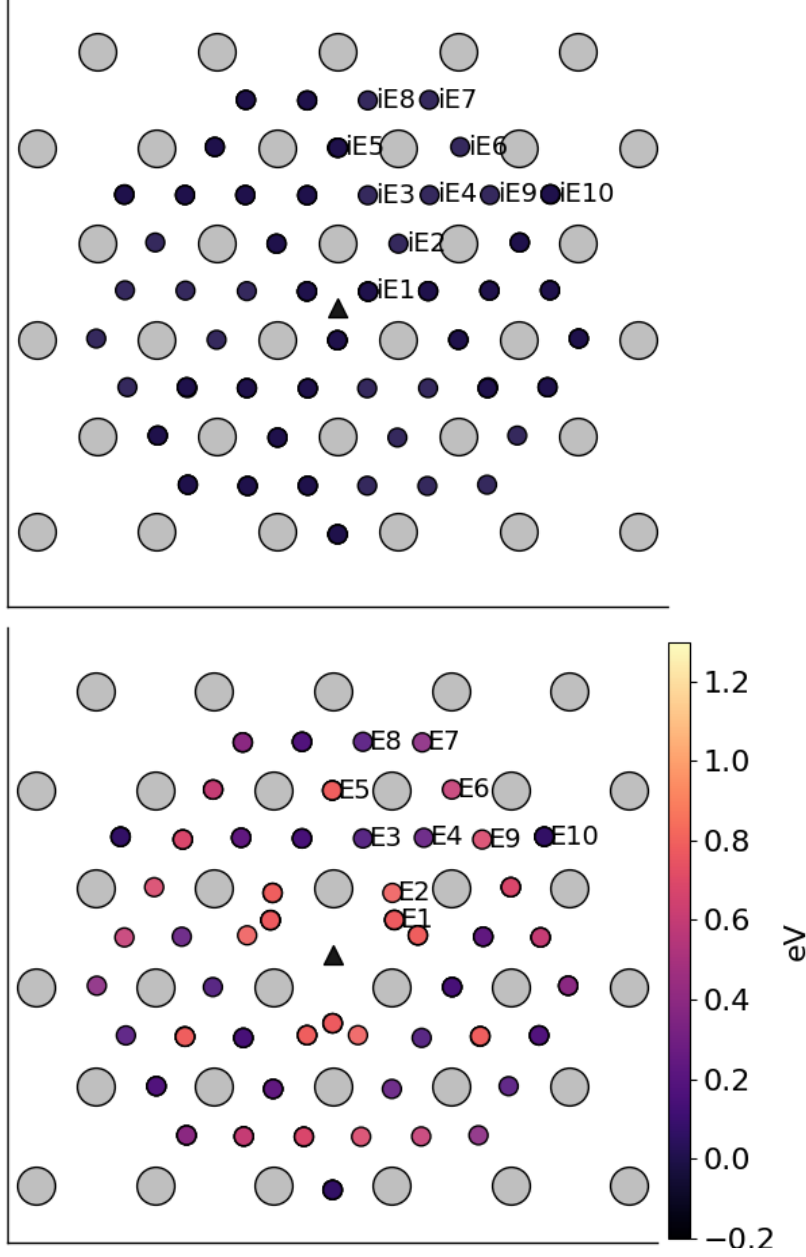


Table 3: Initial and final positions and binding energies (eV) of carbon around the easy core. Binding energies are not shown for the initial positions. Top: initial positions before relaxation. Bottom: final positions and binding energies after relaxation. The core was constrained by fixing the top and bottom three atoms surrounding each of the cores. As shown by Ventelon [5], the first and second closest octahedral sites to the hard core decay to a prismatic position inside the hard core.

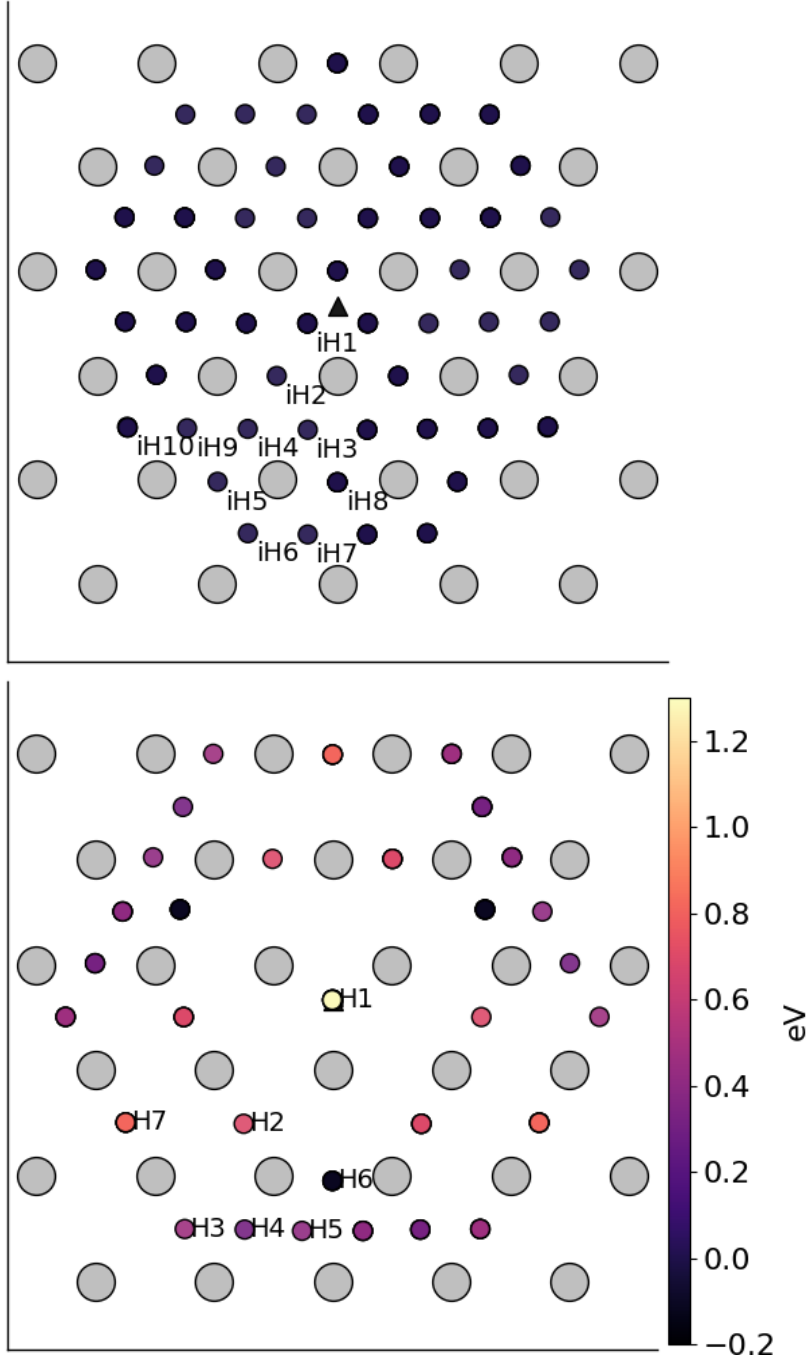


Table 4: Final positions and binding energies (eV) of carbon around the hard core. Top: initial positions before relaxation. Bottom: positions after relaxation. The core was constrained by fixing the top and bottom three atoms surrounding each of the cores. As shown by Ventelon [5], the first and second closest octahedral sites to the hard core decay to a prismatic position inside the hard core.

Site Type	distance from core [b]	E^z [eV]	ΔE^z [eV]	E_b [eV]	E_b^z [eV]
E1	0.57	0.185	-0.018	0.793	0.775
E2	0.70	0.202	-0.001	0.793	0.793
E3	0.99	0.205	0.002	0.137	0.139
E4	1.21	0.208	0.005	0.229	0.234
E5	1.36	0.210	0.008	0.784	0.791
E6	1.66	0.209	0.007	0.597	0.603
E7	1.89	0.206	0.003	0.385	0.388
E8	1.77	0.203	0.000	0.177	0.178
E9	1.52	0.201	0.000	0.683	0.683
E10	1.95	0.202	0.000	0.067	0.067
H1	0.00	0.196	-0.006	1.298	1.291
H2	1.19	0.210	0.007	0.691	0.698
H3	2.12	0.209	0.007	0.461	0.467
H4	1.91	0.207	0.005	0.311	0.316
H5	1.80	0.208	0.006	0.403	0.409
H6	1.40	0.207	0.005	-0.119	-0.114
H7	1.35	0.206	0.006	0.825	0.819

Table 5: Table of energies leading to the zero-point energy corrected binding energy using the cluster method for simulation of dislocation-carbon interactions.

with the continuum limit of Eshelby theory with a binding energy of 0.2 eV.

In work by Ventelon [5], the interaction energy of a carbon in a hard core prism configuration was found to be 0.79 eV for a thickness in the Z direction of $3b$ (0.73eV for $6b$)—in the convention that a positive binding energy indicates attraction. This is significantly lower than the 1.29eV interaction energy of tight-binding.

This discrepancy can be partially explained by the fact that the cells have not been allowed to relax with all degrees of freedom, as in the Ventelon results: the three atoms around the screw core are fixed in Z to fix the dislocation core position. A larger source of error is likely to do with the fitting of the tight-binding model itself. The Peierls barrier of this s-d model of iron, necessary for Fe-C interactions, has been show to be half that found in DFT, or the canonical d model [10], but the solution energies for Fe-C defect complexes are well described. This implies there is insufficient repulsion between Fe-Fe species, upon deformation, leading to a higher Fe-C binding energy from tight-binding, compared to DFT.

Analysing these results, one can predict the equilibrium carbon concentration of a given carbon binding site, assuming carbon atoms around the core are sufficiently spaced such that intersite interaction energies are negligible [5].

The fraction is given by

$$\frac{c_d^i}{1 - c_d^i} = \frac{c_{\text{bulk}}}{1 - c_{\text{bulk}}} \exp\left(-\frac{E_b^i}{k_B T}\right),$$

where i denotes the i^{th} carbon binding site, with E_b^i , being the corresponding dislocation-solute binding energy and c_d^i being the concentration that carbon site on the dislocation. c_{bulk} is the carbon concentration in the bulk, with c_{nom} the nominal carbon concentration per Fe atom.

In a volume V , the number of carbon sites along the dislocation cores is $N_d = \rho V/b$, with ρ the dislocation density, while the number of octahedral sites is $N_{\text{oct}} = 6V/a_{\text{bcc}}$. This gives constraints on the carbon concentrations: $N_{\text{oct}}c_{\text{bulk}} + N_d c_d = N_{\text{oct}}c_{\text{nom}}/3$, where the factor of 3 arises from there being three octahedral sites per Fe atom.

$$C_d^i = \frac{\frac{1}{3}C_C^i \exp\left(\frac{E_b^C}{k_B T}\right)}{1 + \frac{1}{3}C_C^i \exp\left(\frac{E_b^C}{k_B T}\right)},$$

Using Mclean's isotherm to calculate the equilibrium concentration of carbon at normal operating temperatures of bearing operation, C_d ,

$$C_d = \frac{\frac{1}{3}C_C \exp\left(\frac{E_b^C}{k_B T}\right)}{1 + \frac{1}{3}C_C \exp\left(\frac{E_b^C}{k_B T}\right)},$$

The factor of $\frac{1}{3}$ is due to there being 3 octahedral sites per Fe atom.

The binding energy of carbon to dislocations is much greater than that of hydrogen ($E_b^{\text{C}, \text{max}} = 1.29$ eV $E_b^{\text{H}, \text{max}} \approx 0.4$ eV, with hydrogen also in a prismatic-like site). As such, one would expect the drag forces upon the dislocation to be much larger, implying a larger stress is necessary for the dislocation to initially move.

The julia implementation of the NEB/string algorithms was used [14]. One finds that the line shapes are similar to that of Itakura.

4 Discussion

- How do the results of this work feed into C migration with dislocations?
- How valid is the theory we have vs Fu *et al.*
- Novel work to find out dislocation environment around both dislocation cores.

As in [15], carbon interactions are found to be vital in understanding how screw dislocations move in steels. Due to the spontaneous reconstruction of

the easy core upon introduction of carbon, and the large binding energy of the H1 site, one would expect a hard core with carbon in a prismatic site as the ground state configuration for pinned dislocations. With stress, the dislocation will be forced to move (say, along the $X = \bar{2}11$ direction), which results in the hard core reconstructing to an easy core. Due to the much higher velocity of dislocations, relative to the diffusivity of carbon, one expects carbon in the prismatic site will not move, becoming an E1 site. A drag force acting on the dislocation now hinders further motion due to the binding of the carbon in the E1 site relative to the dislocation centre. Progression of dislocation glide results in further reconstruction of the dislocation core to hard, easy and hard cores, with the original carbon being situated in H2, E6 and H3 sites respectively, relative to the dislocation. Thus as the dislocation moves, the drag forces on the dislocation decrease.

This forms the basis of the line tension model of the dislocation. We have a more sophisticated method of being able to incorporate the binding energy of carbon to dislocations than Itakura.

- Peierls potential agrees, although it is low compared to DFT
- Line tension model has been set up, although results have not been achieved yet.
- kMC depends on the results of the line tension model.

The first stage in this work is

5 Future work

- Validation of line-tension model by reproduction of the dislocation line shape from Itakura 2012 [7].
- Compare the dislocation line shape with Itakura, and find the migration path of the dislocation from the data.
- [Optional] Create Ising model for easy and hard core and compare the binding energies like [15].
- [Optional] Find the elastic dipole tensor to check the binding energy of C within anisotropic elasticity.
- Choose the sites for which one can fit a function (lorentzian) for the interaction energy between C and Fe.
- Find the kink-pair formation enthalpy, with and without carbon, to feed into the kMC code.

It would be of interest to pursue atomistic calculations of carbon bound to edge dislocations. Recent work by Maugis *et al.* [16], show that, counterintuitively, under *compressive* stress, carbon diffusivity is *enhanced*. Pipe diffusion of carbon along edge dislocations could therefore be a very important aspect of dislocation-assisted carbon migration.

6 Conclusion

- Outline of the literature review
 1. Origin of DER formation through high-cycle fatigue
 2. What is the DER region and what phases is it composed of?
 3. What are the current mechanisms which explain this?
 - (a) Why are they insufficient?
 4. Outline of the work considering Fe-C dislocation modelling

7 Appendix

7.1 Regularisation of interaction energy in quadrupolar array

In isotropic elasticity, the elastic energy of a single dislocation dipole in an infinite lattice is given by

$$E_{\text{el}}^{\infty} = \frac{\mu b^2}{4\pi} \ln\left(\frac{r}{r_c}\right)$$

The contribution from periodic images to the correction is

$$E_{\text{img}} = E_{\text{el}}(\mathbf{a}, \mathbf{c}_i, r_c) - E_{\text{el}}^{\infty}(\mathbf{a}, r_c),$$

"Ghost" dipoles are introduced to account for the conditional convergence of the sum at $\pm\alpha\mathbf{b}$ and $\pm\beta\mathbf{b}$, where $\alpha = \beta = 0.5$. We define $E_{\text{dg}}(\mathbf{R})$ as the interaction energy of a ghost dislocation and a dipole at \mathbf{R} anisotropic elasticity equations as shown in [17].

Defining,

$$E_{\text{dd}}(\mathbf{R}) = \frac{\mu b^2}{2\pi} \ln \frac{|\mathbf{R}|^2}{|\mathbf{R} + \mathbf{a}| \cdot |\mathbf{R} - \mathbf{a}|},$$

we obtain,

$$E_{\text{img}} = \frac{1}{2} \sum_{\mathbf{R}} [E_{\text{dd}}(\mathbf{R}) - E_{\text{dg}}(\mathbf{R})] - \frac{1}{2} E_{\text{dg}}(\mathbf{R} = 0),$$

which can be subtracted from the total energy as given from atomistic calculations, for a regularised interaction energy.

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