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Atomistic examination of the unit processes and vacancy-dislocation interaction in dislocation climb

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Atomistic analyses of thermodynamic and kinetic barriers to the unit processes of dislocation climb in body-centered cubic iron are presented. Binding of vacancies to the core is demonstrated to be equivalent to particle adsorption, thereby reducing the number of independent barriers to unit climb. The extent to which vacancy energetics are poorly predicted by elasticity theory of dislocation strain fields near the core, as well as the deviation of migration barriers near versus far from the core, are also quantified.

Keywords: Dislocation; Vacancy; Diffusion; Creep

Fundamental understanding of dislocation climb, the nonconservative motion of line defects out of slip planes via vacancy diffusion to the dislocation core, is key to the study of crystalline deformation mechanisms such as "power-law" creep [1]. However, studies of how vacancy-dislocation interaction energetics at the core deviate from elasticity predictions [2] and of how the vacancy diffusion barrier varies with distance from the core have been largely neglected, due to the difficulty of incorporating these atomistic details into analytical treatments of climb [1,3]. Such realistic complexity could be included in more refined numerical treatments of climb kinetics capable of including these details (either atomistic transition state theory-based techniques, such as kinetic Monte Carlo, or continuum transport equation-solving methods, such as the finite element method), and would facilitate subsequent modeling and simulation of interstitial and substitutional atoms' effects on climb of defected alloys.

Here, we examine the unit processes of dislocation climb for an edge-like mixed dislocation in body-centered cubic (bcc) Fe. We demonstrate that the vacancy binding to the dislocation core can be conceptualized as a particle adsorption phenomenon to significantly simplify the study of vacancy interactions within the core region. We also present the thermodynamic and kinetic parameters of vacancy migration processes, and illustrate how deviations from mobility within the undefected bulk crystal can be tractably incorporated into numerical simulations of climb. Clouet has recently computed the single vacancy energetics as a function of distance from the dislocation core with empirical potentials for a variety of face-centered cubic (fcc) metals [4] and compared the results with elasticity theory. We build upon that perspective to obtain the effect of multiple vacancies in the core and the variation of the vacancy migration barrier as a function of distance from the core in a bcc metal.

For these simulations, we employed our recently constructed Finnis–Sinclair-type empirical potential for bcc Fe, which is capable of duplicating the energetics of many point defect cluster configurations computed from density functional theory [5]. We implemented the $\langle 1\,1\,1\rangle$ $(1\,1\,0)$ 71° mixed dislocation (M111 in the standard notation of Vitek [6]) to facilitate atomistic simulations of an edge-type dislocation with periodic boundary conditions for a reasonable system size and associated computational expense. A monoclinic periodic supercell was constructed with boundaries in the directions of $[1\,1\,1]$, $[\bar{1}\,1\,\bar{1}]$ and $[\bar{1}\,0\,1]$, extending over 40, 10 and 40 lattice layers, respectively. Dislocations were generated by removing planes of atoms along the line direction of $[\bar{1}\,1\,\bar{1}]$ (similar to the dislocation generation method employed in Ref.

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[7]). To simulate the dislocation quadrupole array, the $40 \times 10 \times 40$ supercell was mapped to a new supercell that contained only half as many atoms [8]. Two different dislocation core configurations are necessarily present in our constructed quadrupolar dislocation array described above, as illustrated in Figure 1. We refer to the atom-centered dislocation as AD (the M111 structure as identified by Yamaguchi and Vitek [9]) and the bond-centered dislocation as BD. In a separate dipole calculation (which permits isolation of each dislocation type) we confirmed that both structures are stable and found that the AD is slightly more energetically favorable than the BD by 7.07×10^{-14} J m^{-1}. In this work we chose to focus on the AD core explicitly.

All structural and supercell relaxations were performed by using the conjugate gradients method (CG) as implemented in the GULP code [10]. The minimum energy paths between these energetically minimized structures were computed with the nudged elastic band (NEB) method [11] implemented in gulp. Throughout this work the interaction energy between the Nth vacancy and a dislocation with $N-1$ vacancies is defined as:

$$E_{V\text{-}D}^{inter} = (E + E_{V\text{-}D}) - (E_D + E_V) \quad (1)$$

where E, E_V, E_D and $E_{V\text{-}D}$ refer to the energies of the pure bulk, of the bulk with one vacancy, of the dislocation simulation cell with $N-1$ vacancies and of the dislocation simulation cell with N vacancies [4]. A negative value of $E_{V\text{-}D}^{inter}$ thus indicates vacancy attraction to the dislocation core.

At the atomistic level, the unit process of climb is initiated by the binding of a vacancy to the core, and climb of a given segment is complete when enough vacancies bind to the core to move the entire dislocation line one step normal to the glide plane. We find that significant variation exists among the incremental binding energies of the vacancies to the dislocation core that initiate, continue and complete the climb event. The results are summarized in Table 1, which indicates that the interaction energies range from -109 to -211 kJ mol^{-1}, with a mode of -175 kJ mol^{-1}. (The -109 kJ mol^{-1} required for the initial binding can be compared with -89 kJ mol^{-1} [12] obtained for the edge dislocation.) This provides a further simplification in dislocation climb simulations; namely, the binding of vacancies to the core during climb may be modeled by three separate events: the creation of a jog by the binding of a vacancy to the dislocation core (Fig. 2a), the increase in jog length by an additional vacancy bonding to the line of vacancies in the core (Fig. 2b) and the union of two different jogs (Fig. 2c). These trends illustrate the particle absorption nature of vacancy binding to the dislocation core and could be rationalized as a surface change within the dislocation core. The first vacancy that joins the dislocation core and forms the double kink introduces extra line length or "surfaces" (with the length scale of a nearest neighbor distance) along the line direction and also creates two terminal jog surfaces normal to the dislocation line direction. Subsequent vacancies joining the core continue to expand the jog, adding surfaces along the dislocation line but leaving the number of terminal jog surfaces unchanged. The last vacancy that joins the dislocation core and unifies two jogs adds surfaces along the dislocation line, but also removes the two terminal jog surfaces at either end of the jogged segment. While this conceptualization grossly simplifies the exact nature of vacancy binding to the dislocation core,

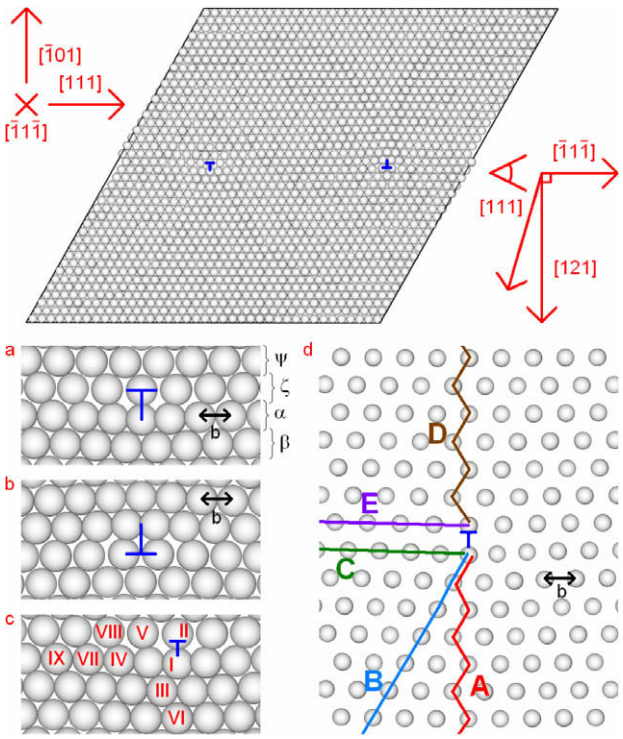

Figure 1. Quadrupolar system containing two different dislocation core configurations: (a) an atom-centered core (the Greek letters in define planes referred to in subsequent discussions); (b) a bond-centered core; (c) various positions around the core as referred to in Table 2; and (d) five (A, B, C, D and E) possible pathways of vacancy movement towards the core referred to in the text. Rendered via AtomEye [14].

Table 1. Interaction energy of dislocation core with N vacancies already bound to the core with a single free vacancy in bulk.

N	$E_{v\text{-}d}$ (kJ mol^{-1})	N	$E_{v\text{-}d}$ (kJ mol^{-1})
0	−109	5	−175
1	−194	6	−176
2	−179	7	−174
3	−176	8	−172
4	−175	9	−211

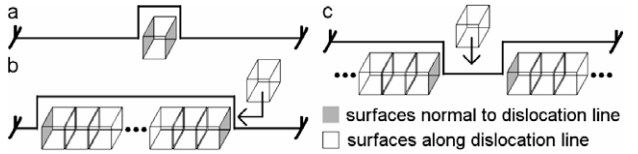

Figure 2. Atomistic schematic of climb: (a) the initiation of a jog by the binding of a vacancy to the dislocation line; (b) the expansion of the jog by binding of vacancy to the ends of a line of vacancies in the core; and (c) the union of two discrete jogs. The line direction of the dislocation system in this work is [$\bar{1}$1$\bar{1}$].

it is consistent with our calculations in two ways. First, from the consideration of the surfaces created, the energy required to increase the jog length by the bonding of one vacancy to the line of vacancies in the core should be equal to half of the sum of energy of initiating the jog (here, -109 kJ mol^{-1}) and of the energy of the union of two jogs (here, -211 kJ mol^{-1}), or -160 kJ mol^{-1}. This estimate agrees well with the calculated result of -175 kJ mol^{-1}. Secondly, this model also predicts that the energy released when a vacancy joins two distinct jogs to form a single, longer jog should exactly match the energy released when a climb event is completed. We obtained the energy of the binding of a vacancy to two adjacent jogs of two vacancies each to form a jog of five vacancies as -225 kJ mol^{-1}. This agrees reasonably well with that calculated for the completion of a climb event (-211 kJ mol^{-1}), confirming the validity of the approximation.

As there are 10 lattice layers along the dislocation line direction of $[\bar{1}\,1\,\bar{1}]$ in our supercell, there are 10 values in the table.

Difficulties in the fundamental understanding of dislocation climb are due to the slow dynamical nature of this collective process; explicit treatment of the nature of dislocation climb ought to address the energetic details (both thermodynamic and kinetic) of vacancies as a function of distance from the core. As shown in Figure 3 for a specific vacancy diffusion path (path A in Fig. 1d), we found that the energetic minima of one single vacancy at different lattice site distances from the dislocation core can be described well by both isotropic [2] and Stroh anisotropic [13] elasticity theories, provided the vacancy and dislocation core are far apart (here, four Burgers vectors). This success of elasticity theory in predicting vacancy energetics at nearest neighbor differences is in qualitative agreement with Clouet's observations for fcc metals [4]. Figure 3 also indicates that, in the region where the elasticity theory assumption holds, the interaction energy is typically small ($\sim$5 kJ mol^{-1}). This trend is consistent with the results of Kamimura et al. [12] for the edge dislocation type (in the notation of Vitek [6]) using the same empirical potential. This result shows that vacancies interacting with edge-type dislocation cores can be treated as free vacancies subjected to the elastic field of a dislocation. Explicit atomistic treatment is necessary only when vacancies are a few Burgers vectors away from the core, as is well established by the principle of the core cut-off radius in elastic treatment of dislocations.

As shown in Figure 3, the migration barriers of the single vacancy towards the core converges to the vacancy migration barrier in the perfect lattice at approximately four Burgers vector distances from the dislocation core. Similar trends are found for the other four migration paths specified in Figure 1, with relevant variations highlighted in Figure 4a. The vacancy migration barriers for diffusion parallel to the dislocation line length show similar behavior as well (Table 1). We note that the significant differences between the paths imply that any attempt to model the near-core vacancy behavior should not ignore the angular dependence of the paths in relation to the core that is neglected for purposes of simplification in analytic studies of climb [1,3].

It is also of interest to investigate cases of the migration energies of vacancies toward jogged dislocation segments (i.e. vacancies are bound to the core). Taking Path A as an example, we identify three variations that arise from the loss of translational symmetry along the dislocation line as a result of the presence of vacancies within the core (Fig. 4c): two for the extension of the jog by vacancy binding (AI and AII) and one for uniting two jogs (AIII). The results of the vacancy energetics along the paths can be seen in Figure 4b. We observe that the barriers of migration to the core only vary significantly from the monovacancy case within one nearest neighbor distance from the core. This result suggests that perturbations within the core have a very short range effect, as compared to the dislocation strain field itself, on the energetics of vacancies approaching the core. Such quantitative observations significantly reduce the amount of information needed to be tabulated from atomistics and transferred to kinetic simulations, as the kinetics of the monovacancy case can be used to be representative of the general vacancy interactions with jogged or unjogged dislocation segments, except for

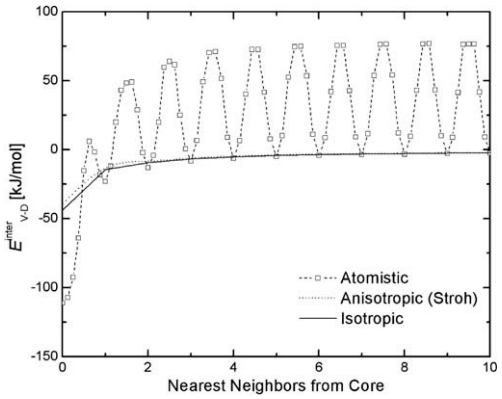

Figure 3. Vacancy and dislocation core interaction energy as a function of the number of nearest neighbor jumps of the vacancy away from an otherwise "pure" dislocation core in Path A, relative to a vacancy in a pure bulk. Values at whole numbers of jumps represent the energies of vacancies at an atomic site obtained by conjugate gradients minimization. These are to be compared with the predictions of elasticity theory and with the findings of Clouet [4]. We further include the energy barriers that arise from movement of the vacancy between discrete lattice points, where the points between whole numbers jumps represent the minimum energy path for the jump obtained by the NEB method and the peaks correspond to the migration barriers. For reference, the migration of the vacancy in bulk is 81 kJ mol^{-1} [5].

Table 2. The migration energy of vacancies parallel to the dislocation line direction of $[\bar{1}1\bar{1}]$ at various positions around the core as defined in Figure 1c, and the convergence seen for the migration towards the core towards the bulk migration energy of 81 kJ mol^{-1} [5] within four Burgers vector distances from the core.

Position	$E_{barrier}$ (kJ mol^{-1})	Position	$E_{barrier}$ (kJ mol^{-1})
1	124	VI	81
II	83	VII	68
III	68	VIII	86
IV	55	IX	76
V	93		

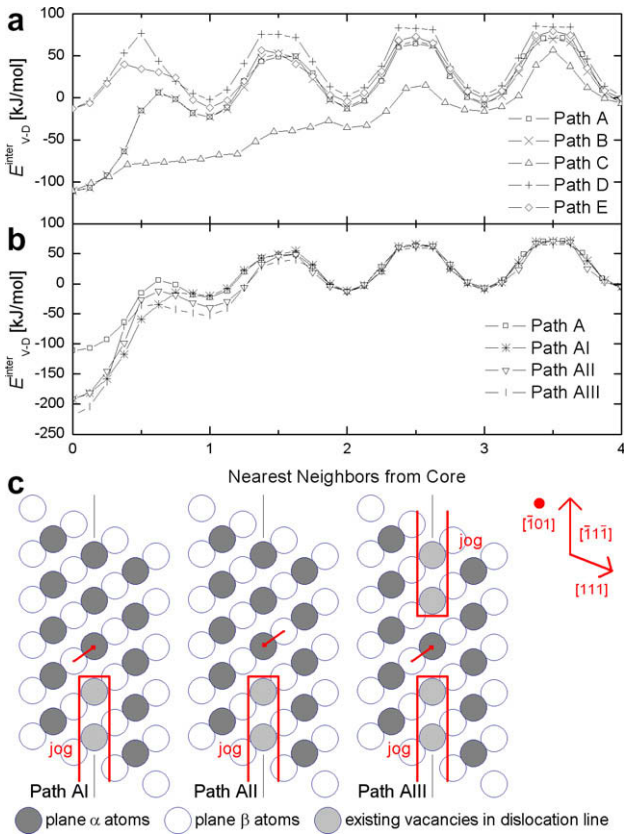

Figure 4. (a) Interaction energy of a pure dislocation and a single vacancy as a function of the number of nearest neighbor jumps of the vacancy away from an otherwise unjogged dislocation core for paths specified in Figure 1, relative to a vacancy in a pure bulk. The points between whole numbers of jumps mark the vacancy migration energies. Note that Paths A, B and C are on the compressive side of the dislocation core, while Paths D and E are on the tensile side of the dislocation core. The difference between the compressive and tensile nature gives rise to two distinct values for E^{inter}_{V-D} at the 0th nearest neighbor from the core. (For reference, the vacancy migration barrier from the core position on the compressive side to the core position on the tensile side, i.e. from position I to position II in Figure 1, is 167 kJ mol^{-1}.) (b) Interaction energy between an unjogged dislocation segment and a single vacancy versus the number of nearest neighbor jumps of the vacancy away from an otherwise unjogged dislocation core in paths specified in (c), relative to a vacancy in a pure bulk. For Paths AI and AII, the vacancy joins another vacancy in the core to form a line of two vacancies at the core. For Path AIII, the vacancy joins two separate lines of two vacancies each to form a continuous line of five vacancies in the core. The energetics of the single vacancy traveling on Path A are included as well for comparison. (c) Paths AI, AII and AIII referred to in (b). See to Figure 1a for the definitions of paths and planes.

interactions in which the vacancy is one nearest neighbor from the dislocation core.

In summary, we have presented a systematic analysis of the unit processes of dislocation climb for a mixed dislocation in bcc Fe. We draw three general conclusions about the vacancy interaction with and migration behavior near a dislocation core. First, the vacancy core binding energetics can be approximated as an adparticle modification of the dislocation core. Secondly, significant differences in the energetics and migration barriers of the vacancies around a dislocation core from the free vacancy occur in a vicinity of a few Burgers vector $|\vec{b}|$ distances from the core ($4|\vec{b}|$ for this dislocation in bcc Fe). Thirdly, the energetics and migration barriers of the monovacancy binding to the core can be taken as representative of vacancy binding to a jogged core containing an arbitrary number of vacancies, except in the very last unit process of vacancy binding directly to core. These observations can be directly applied to numerical treatment of the kinetics of dislocation climb, and the general approach and methodology can be used in studies of dislocation interactions with other defects (e.g. solute atoms).

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[1] J. Weertman, J. Appl. Phys. 26 (1955) 1213.
[2] J.P. Hirth, J. Lothe, Theory of Dislocations, McGraw-Hill, New York, 1968.
[3] W.D. Nix, R. Gasca-Neri, J.P. Hirth, Philos. Mag. 23 (1971) 1339.
[4] E. Clouet, Acta Mater. 54 (2006) 3543.
[5] T.T. Lau, C.J. Först, X. Lin, J.D. Gale, S. Yip, K.J. Van Vliet, Phys. Rev. Lett. 98 (2007) 215501.
[6] V. Vitek, Cryst. Lattice Defects 5 (1974) 1.
[7] S. Simonetti, M.E. Pronsato, G. Brizuela, A. Juan, Appl. Surf. Sci. 217 (2003) 56.
[8] J.R.K. Bigger, D.A. McInnes, A.P. Sutton, M.C. Payne, I. Stich, R.D. King-Smith, D.M. Bird, L.J. Clarke, Phys. Rev. Lett. 69 (1992) 2224.
[9] M. Yamaguchi, V. Vitek, J. Phys. F 3 (1973) 523.
[10] J.D. Gale, A.L. Rohl, Mol. Simul. 29 (2003) 291.
[11] H. Jónsson, G. Mills, K.W. Jacobsen, in: B.J. Berne, G. Ciccotti, D.F. Coker (Eds.), Classical and Quantum Dynamics in Condensed Phase Simulations, World Scientific, Hackensack, NJ, 1998, pp. 385–404.
[12] Y. Kamimura, T. Tsutsumi, E. Kuramoto, Phys. Rev. B 52 (1995) 879.
[13] A.N. Stroh, Philos. Mag. 3 (1958) 265.
[14] J. Li, Modelling Simul. Mater. Sci. Eng. 11 (2003) 173.