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Acta Materialia 55 (2007) 93–104

Acta MATERIALIA

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Computer simulation of interaction of an edge dislocation with a carbon interstitial in α-iron and effects on glide

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Received 18 April 2006; accepted 8 August 2006
Available online 3 November 2006

Abstract

The atomic-scale behaviour of a carbon (C) interstitial atom in the core of a $1/2[111](1\bar{1}0)$ edge dislocation in α-iron has been simulated for the first time. C sites with high binding energy to the dislocation have been investigated and the critical stress, τ_c, for the dislocation to overcome a row of C atoms determined. The effects of temperature, T, and applied strain rate, $\dot{\varepsilon}$, on τ_c have been studied. τ_c decreases rapidly as T increases to ~400 K and becomes almost constant at higher T. It decreases with decreasing $\dot{\varepsilon}$ and is $\dot{\varepsilon}$-independent at T greater than ~300 K. The activation parameters in simulation conditions have been obtained. The activation distance of ~(0.2–0.3)b is consistent with point-obstacle strengthening. However, the activation energy is only $\sim 5k_BT$, where k_B is the Boltzmann constant, and $\sim 20k_BT$ smaller than that realized in experimental conditions. This implies that the decline of τ_c over the range 0 to ~400 K would occur over 0 to ~80 K in experiment, which is where C-edge dislocation effects would be influential. A few jumps of C occur in the core before dislocation unpinning at $T \geqslant 800$ K and give a small T-dependence of τ_c. Core diffusion of C occurs by $\pm 1/2[11\bar{1}]$ jumps at 70.5° to [111]. The diffusivity in the absence of applied stress is $4\times10^{-9}\exp(-0.2\ \mathrm{eV}/k_BT)\ \mathrm{m^2/s}$ compared with $1.9\times10^{-7}\exp(-0.7\ \mathrm{eV}/k_BT)\ \mathrm{m^2/s}$ for bulk diffusion of C in the same MD model. Hence, the edge dislocation provides a path for rapid diffusion of C, but net transport along the core can only occur by motion of the dislocation itself.

Keywords: Dislocation mobility; Carbon diffusion; Iron alloys; Molecular dynamics; Activation parameters

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1. Introduction

The properties of carbon in iron have been investigated extensively because of its relevance to steel technology. It is known from experiment that the interaction of C interstitial solute atoms with lattice defects significantly affects mechanical properties of ferritic steels, e.g. their strength [1], and the apparent properties of point defects such as vacancies [2,3]. Carbon has small solubility (0.002 wt.%) in the α-Fe matrix at room temperature. Above the solubility limit, it precipitates as carbides or cementite (Fe_3C) in pearlite, which is useful for improving the strength of steels. In quenched irons, C is retained in martensite. C atoms that remain in solution in ferrite can also have a significant influence on steel properties by their interaction with lattice defects, e.g. acting as traps for vacancy-type defects and thus decreasing the vacancy diffusion coefficient [2,3]. The migration properties of C atoms in α-iron and their interaction with intrinsic point defects have been investigated experimentally, e.g. by positron annihilation [3], and theoretically, e.g. by molecular dynamics [4] and by means of *ab initio* calculation [5]. Furthermore, first-principles calculation [6] and experiment [7–9] provide evidence that C is a cohesion enhancer at grain boundaries in Fe.

In the context of the present paper, the interaction between C impurity and dislocations is particularly important. It can have significant impact on the mechanical properties of steel by its influence within the dislocation core. At

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doi:10.1016/j.actamat.2006.08.015

high enough temperature, solute C atoms can diffuse to a dislocation and form a C-rich atmosphere (the 'Cottrell atmosphere' [1]). Core segregation of C immobilizes dislocations and increases the applied stress required for them to take part in yielding. Even without the ageing process that leads to atmosphere formation, C in solution is believed to offer strong resistance to dislocation glide.

Variations on the elasticity model of the interaction energy, E_I, between an edge dislocation and a C atom have been proposed by several workers (e.g. [1,10–14]). These describe the far-field interaction, but elasticity provides only an approximation for C sites near the dislocation core and so atomic-level computer simulation should be employed for this region [15–17]. In an early study, de Hosson [15] simulated the interaction of a C atom and a $1/2[111](1\bar{1}0)$ edge dislocation using the pairwise interatomic potentials for Fe–Fe derived by Johnson [18] and Fe–C by Johnson et al. [19]. The results showed that C atoms with maximum binding to the dislocation lie between the $\{110\}$ atomic planes immediately under the extra half-plane where E_I is -0.7 eV, which is consistent with elasticity estimates. Recently, Niu et al. [16] and Simonetti et al. [17] investigated electronic effects of C in the core of $\langle 100\rangle$ and $1/2\langle 111\rangle$ edge dislocations in α-iron by *ab initio* methods based on density-functional theory. It was found that a C atom can weaken interactions between the adjacent Fe atoms and form strong covalent-like bonds with them, thereby leading to carbon–dislocation complexes.

In the present work, the interaction of carbon interstitials with an edge dislocation in dilute Fe–C alloy and their effect on the motion of the dislocation are investigated. Molecular statics (MS) and molecular dynamics (MD) techniques are employed to simulate conditions with temperature $T = 0$ K and $T > 0$ K, respectively. These methods require interatomic potentials in order to compute potential energy of atoms and forces on them. The development of empirical interatomic potentials for computer simulation of C in α-Fe has lagged behind that for pure α-Fe and Fe alloys with substitutional solutes, and only a few Fe–C potentials have been proposed. Johnson et al. [19] developed a short-range pair potential set for the Fe–C system by fitting to the experimental value of 0.86 eV for the migration energy of C atoms in α-Fe [20], zero activation volume of migration [21] and vacancy-carbon binding energy of 0.41 eV. C–C interaction was not considered in this model. This potential, which was used by de Hosson [15], reproduces the experimental value of the energy of solution of a C atom in α-Fe relative to that in Fe_3C [22] and gives the octahedral site as the most stable one for a C interstitial, consistent with experiment [23] and subsequent *ab initio* calculation [5]. Although the volume expansion due to a C atom is ~0.3Ω, where Ω is the Fe atomic volume, compared with ~0.8Ω deduced from the experimental value of lattice parameter change with C composition [24], the relaxation of Fe atoms neighbouring a C atom obtained in Ref. [4] by a combination of the Fe–C potential of Johnson et al. and many-body Fe–Fe potentials (either the Finnis–Sinclair (F–S) potential of Ackland et al. [25] or the embedded-atom method (EAM) potential of Ackland et al. [26]) is in good agreement with that found in a recent *ab initio* calculation by Domain et al. [5]. There have been several attempts to obtain a better description of C atoms in iron using empirical potentials. Rosato [27] rescaled the Fe–C potential of Johnson et al. [19] to use with an FS-type many-body potential for Fe [28], which provides a better description of the elastic properties of α-Fe than the simple Fe–Fe pair potential in Ref. [19]. Again, C–C interaction was ignored. Although the octahedral site is the most stable for C in this model, the carbon migration energy is found to be 1.14 eV, which is too high. Ruda et al. [29] developed EAM potentials fitted to *ab initio* data for metastable Fe–C carbide with B1 structure. The C–C interaction was described using the Tersoff [30] potential with no angular dependency. The equilibrium lattice constant, bulk modulus and cohesive energy of stable and metastable carbides were reproduced, but, in contradiction with experiment and *ab initio* calculation, the tetrahedral site is the most stable position for a C atom in α-Fe with this potential. Lee [31] has developed very recently a modified EAM potential for Fe–C. It produces a CV binding energy of 0.9 eV, which is close to that predicted by Vehanen et al. [3] (i.e. 0.85 eV), but much higher than the value of 0.41 eV deduced by Arndt and Damask [32], which was used to fit the Fe–C potential of Johnson et al. [19], and the *ab initio* value of 0.47 eV [5]. It gives a large binding energy (0.68 eV) between C and a self-interstitial atom, as do all the empirical potentials, e.g. 0.58 eV with the model used in the present work, compared with -0.19 eV by *ab initio* calculation. This is an anomaly that has not yet been resolved.

Thus, we are not aware of any potential set that accurately represents the Fe–C system, and so the approach adopted here is to use a 'model' system for an octahedral interstitial solute in a bcc metal matrix that has many similarities to the real alloy. Fe–Fe interactions are computed from the FS-type many-body potential of Ackland et al. [25], which has been widely used to simulate point and extended defects. This is combined with the pair potential of Johnson et al. [19] for Fe–C. In the absence of a reliable C–C interatomic potential, we treat the dilute concentration limit of only a single C atom interacting with the dislocation within the simulation cell. Despite the simplicity of this approach, the model system has many properties, such as elastic constants, solute site stability, migration energy, neighbour-atom displacements and some intrinsic point defect–solute interaction energy values, that are close to those of the real alloy.

The paper is organized as follows. The parameters and method used are presented in Section 2. E_I for C in sites within and near the dislocation core at 0 K is calculated using MS and presented in Section 3. Section 4 describes the results for the critical resolved shear stress, τ_c, required for the dislocation to overcome a C atom situated in a site