Interactions between carbon solutes and dislocations in bcc iron

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Abstract

Carbon solute–dislocation interactions and solute atmospheres for both edge and screw dislocations in body-centered cubic (bcc) iron are computed from first principles using two approaches. First, the distortion tensor and elastic constants entering Eshelby's model for the segregation of C atoms to a dislocation core in Fe are computed directly using an electronic-structure-based the total energy method. Second, the segregation energy is computed directly via first-principles methods. Comparison of the two methods suggests that the effects of chemistry and magnetism beyond those already reflected in the elastic constants do not make a major contribution to the segregation energy. The resulting predicted solute atmospheres are in good agreement with atom probe measurements.
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1. Introduction

The mechanical properties of ferritic Fe–C alloys such as yield points, ductilities and toughnesses are influenced by the solute atmosphere around dislocations [1]. In addition to lattice friction, solutes may exert pinning forces that further impede dislocation plasticity. Sharp yield points or strain aging results from a static atmosphere at low temperature, while a mobile atmosphere at intermediate temperature results in dynamics strain aging or the Portevin–Le Chatelier effect [2]. Designing new ferritic alloys or other materials depends on the accuracy of probing and predicting the properties of the solute atmosphere.

Imaging the solute atmosphere of C atoms in ferritic Fe–C alloys has been made possible only recently using atom probe tomography [3]. The extent of spreading of the solute atmosphere is of the order of 10 nm, while the enrichment factor, the ratio of the concentration of solute in the neighborhood of the dislocation over the matrix concentration, is approximately 7.7 (within the considered region). Both the extent of spreading and concentration of solute atoms implies that much of the atmosphere resides far from the elastic singularity of the core (the region within approximately one Burgers vector of the core, where bonding topology differs substantially from the bulk crystalline counterparts). In regions remote from the core, elasticity theory should be suitable for predicting defect interactions and carbon solute atmospheres.

The elasticity theory of carbon solute–dislocation interactions has been extensively studied. Cochardt et al. [4] studied the interaction using isotropic linear continuum elasticity theory to describe the dislocations. A similar theory was formulated by Bacon [5], where the tetragonal distortion of the interstitial solute was modeled as an elastic dipole tensor. Anisotropic linear continuum elasticity theory was later employed in the work by Douthwaite and Evans [6]. The most recent published work represents a conjunction of elasticity theory and atomic scale simulations [7].

The maximum solute–dislocation interaction energies from these models are summarized in Table 1. Note that the predicted maximum of the solute interaction energy with screw dislocations based on elasticity theory is about 75% of that for edge dislocations. Also, the variation of

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Table 1
Elasticity theory predictions of solute–dislocation interaction energies. The maximum interaction energy is calculated at $r = |\mathbf{b}|$.

References	Dislocation type	Dislocation models	Distortion type	Maximum interaction energy (eV)
[1]	Edge	Isotropic	Isotropic	–
[4]	Edge, screw	Isotropic	Tetragonal	0.75, 0.75
[5]	Edge, screw	Isotropic	Tetragonal	0.49, 0.37
[6]	Screw	Anisotropic	Tetragonal	0.60
[7]	Edge, screw	Anisotropic	Tetragonal	0.40, 0.30

the maximum interaction energies within these studies varies by more than a factor of 2. Clearly, further detailed theoretical studies of solute–dislocation interaction and solute atmospheres are still needed.

Differences in the maximum interaction energies reported in Table 1 stem from two sources: variations in (1) the assumed elastic constants, and (2) the amount of distortion induced by a carbon interstitial.

Experimentally, there have been attempts to measure the lattice distortion induced by a single solute atom. Typically, the lattice parameter of Fe–C martensite is used to measure the strain. A large variation of data on lattice parameter changes with carbon content has been observed [11]. The scatter arises from experimental errors due to different methods employed for lattice parameter determination and the existence of residual stresses from quenching the austenite that might suppress lattice parameter changes. Another possible source of error is the effect of equivalent interstitial sites. Since carbon atoms can fill one of the three equivalent octahedral sites in body-centered cubic (bcc) iron, the resultant average deformation may trend toward isotropic, rather than tetragonal. Despite these issues, experimental results appear to have converged. Fig. 1 replots the data from Refs. [8–10] as considered and plotted in Ref. [11]. The experiments indicate that the lattice parameters of Fe–C alloys depend linearly on C composition for the studied range.
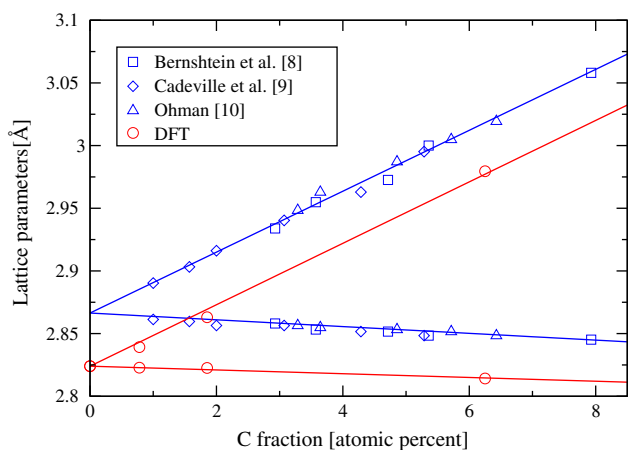

Fig. 1. Least-square fits of lattice parameters (a, c) computed from first-principles as functions of the number of C atoms. The least-square fits of experimental data originally reported in Refs. [8–10], and collected by Cheng et al. [11] are also plotted. The calculated and experimental data are not scaled to the same origin.

Theoretically, the most fundamental study of defect interactions is due to Eshelby [12,13]. Eshelby has shown that the tetragonal solute–dislocation interaction energy is the product of the strength of the point source and the strain field produced at the point source by the dislocation. In this work, we revisit this model and show that Eshelby's formulation can be complemented by first-principles calculations based on density functional theory (DFT) [14]. Specifically, the strength of the point source and the elastic constants entering Eshelby's expressions can be computed directly using electronic-structure-based total energy methods. Further, electronic structure methods can be used to compute the segregation energy directly. This more direct approach yields the correct continuum limit and can, potentially, reveal chemical and magnetic contributions to the interaction beyond those already reflected within the elastic constants and distortion tensor. Further, the direct approach may be extended to high-strain situations, where linear elasticity theory may no longer be valid.

The theoretical basis of the calculations is developed in Section 2. The ab initio calculations and results for a dilute Fe–C alloy are described in Section 3. In Section 4, the theory is used to compute the distribution of C solute atoms around edge and screw dislocations in Fe.

2. Computational approach

Eshelby has shown that by regarding the solute atom as a point source of stress, particularly for one where the forces are unequal along the horizontal and vertical axes [12], the interaction energy of the solute and the dislocation is:

$$F^{int} = -\Gamma_{ij}^{o} \Delta_{ij}^{d}, \qquad (1)$$

where Γ_{ij}^{o} is the strength of the point source, and Δ_{ij}^{d} is the distortional field produced at the source by the dislocation. The strength of the source Γ_{ij}^{o} is the elastic dipole moment of the solute atom [15,16]. It is a function of the electronic structure differences and bonding between the host atoms and the solute atom.

In principle, computing Γ_{ij}^{o} using atomic scale approaches should be straightforward. One simply includes an interstitial atom within an Fe crystal, and measures the displacements of the atoms within the crystal. In practice, however, the procedure is more complex. The best electronic-structure-based total energy methods are computationally expensive and work best for periodic systems.