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Numerical modeling of the core structure of [100] dislocations in Fe_3C cementite

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The core structure of [100] screw dislocation has been modeled in Fe_3C cementite, using the Peierls–Nabarro–Galerkin model based on γ-surfaces for (010) and (001) planes. We show that γ-surfaces and core structure of the [100] screw dislocation depend of the relaxation procedure applied to the carbon atoms during γ-surface calculations. We find that [100] screw dislocations spread in (010) with a tendency toward dissociation, which is in agreement with dislocation features observed experimentally.

Keywords: Cementite; Slip system; Generalized stacking fault energies; Screw dislocation core

Cementite Fe_3C is the main iron carbide in pearlitic steels and plays a pivotal role in determining their strength [1–4]. Cementite exhibits an orthorhombic symmetry. When described within the *Pnma* space group, lattice parameters are $a = 5.09$ Å, $b = 6.75$ Å and $c = 4.52$ Å [5]. A Fe_3C unit cell contains 12 iron atoms and four carbon atoms. Regarding mechanical stability, this material is strongly anisotropic in terms of elasticity and ultimate properties [6,7]. Despite numerous studies on the mechanical properties of pearlitic steels, our understanding of the basic deformation mechanisms of cementite is still incomplete. In a recent study, Kar'kina et al. [8,9] drew attention on the contribution of partial [100] dislocations gliding in (010) in cold plastic deformation of cementite in granular pearlite. The ability of a phase to deform through partial dislocation has profound implications on plastic anisotropy. The presence of dissociated dislocations has also been shown to affect carbon migration kinetics [8]. To further investigate this tendency, Kar'kina et al. [10] conducted molecular dynamics calculations of generalized stacking faults (GSFs, also called γ-surfaces) in cementite. The existence of local minima in the γ-surfaces provides further evidence that dislocation core spreading could strongly constrain the choice of slip systems and plastic anisotropy in cementite. However, there is no model of dislocation core in cementite available so far to establish the easiest slip planes of dislocations.

In the present work, we use the Peierls–Nabarro–Galerkin method [11,12] to model the core structure of [100] dislocations. We focus on dislocations with screw character since the tendency of this dislocation to spread in one or the other plane will have strong implication on the choice of the slip plane and plastic anisotropy. Considering the sensitivity of γ-surface calculations on relaxation conditions [13], especially in phases containing small interstitial elements [14], we have conducted ab initio calculations of GSFs and evaluated the influence of C mobility on their determinations.

First-principles calculations using spin polarization and based on the density functional theory [15,16] have been performed using the Vienna ab initio simulation package (VASP) [17–20]. The projector-augmented wave method [21,22] was adopted for pseudo-potentials and the gradient-corrected functional [23,24] was used for the exchange correlation energy function as implemented in VASP. Following earlier work [6], a plane-wave energy cut-off of 500 eV was used to ensure the convergence of energy. Calculations of (010) and (001) γ-surfaces rely on supercell methods (Fig. 1). Both supercells contain 48 atoms. They were sheared at two different levels labeled *A* and *B* in the (010) plane and α and β in the (001) plane (Fig. 1). We also introduced a 14 Å thick vacuum buffer in the direction normal to the slip plane to avoid interaction between repeated stacking faults resulting from the use of periodic boundary conditions. A reciprocal *k*-point grid size of $9 \times 9 \times 1$, according to the Monkhorst–Pack scheme [25],

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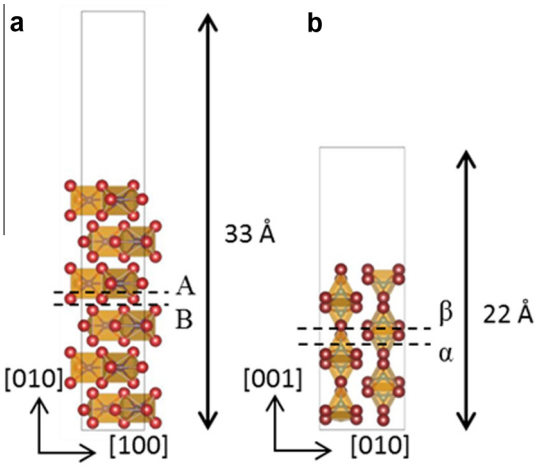

Figure 1. Supercells used for the γ-surface calculations. The vacuum buffer is represented as well as the cutting levels investigated. (a) Shear plane (010); (b) shear plane (001).

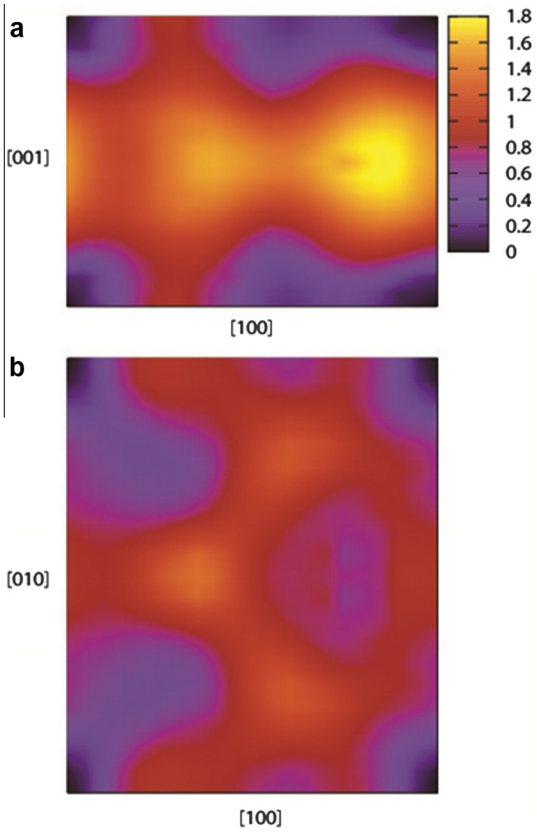

Figure 2. γ-surfaces (in J m^{-2}) calculated ab initio using the full relaxation conditions of the carbon atoms. (a) (010) plane at shear level *A*; (b) (001) plane at shear level α.

was then used to evaluate the generalized stacking fault energies.

Cai et al. [13] have demonstrated the importance played by atom relaxation in the accurate determination of stacking fault energy. In the case of compounds containing carbon atom in interstitial sites, hence potentially mobile, this is particularly important since carbon distribution has been shown to affect the stacking fault energy in Fe–C alloys [14]. To investigate this effect, two relaxation schemes were considered. In the first one, all atoms in the supercell except those located close to the vacuum layer are allowed to relax in the direction perpendicular to the slip plane to minimize the generalized stacking fault energy (further referred to as VR ("vertical relaxation") γ-surfaces). In the second one (called FR ("full relaxation")), carbon atoms are allowed to relax in any direction (this does not apply to the few fixed atoms close to free surfaces). We investigated the possibility of applying shear at different levels, as shown in Figure 1.

γ-surfaces (FR) corresponding to the (010) and (001) planes are presented in Figure 2. Due to the symmetry of the *Pnma* space group, γ-surfaces exhibit a mirror plane along [001] in (010) and along [010] in (001), both containing a maximum of excess energy. In both (010) and (001) planes, the lowest energy paths are found along the [100] direction, emphasizing the importance of [100] as a Burgers vector for further dislocation modeling. In the (001) plane, [100] shear is clearly easier when applied at level α (Fig. 3a). Changing the relaxation conditions for the carbon atoms has little effect on the energy in this plane, as seen in Figure 3a. The (010) plane is more sensitive to the relaxation conditions. Shearing along [100] (010) at the *A* or *B* level leads to excess energies that are comparable. When sheared at the *B* level (Fig. 3b), the [100] (010) γ-line exhibits a first maximum at 30% shear followed by a secondary maximum at 75% shear with, in between, an unstable stacking fault (local minimum of the excess energy) located at 60% of the shear displacement. This aspect is preserved whatever the relaxation conditions applied to the carbon atoms. Allowing their full relaxation, however, leads to lower energies for both the barriers and the unstable stacking fault, which goes from 0.45 J m^{-2} (VR) to 0.21 J m^{-2} (FR). Allowing full relaxation of carbon has more influence on the general aspect of the γ-line corresponding to a cut at the *A* level (Fig. 3c). The smallest energy barrier on the right-hand side decreases strongly, cancelling the unstable stacking fault, which was already less prominent at this level. The efficiency of the FR relaxation scheme in decreasing the energy landscape is linked to the distance between the glide plane and the carbon atoms in the supercell.

In this study, the [100] screw dislocation core is modeled by the Peierls–Nabarro–Galerkin method [11,12], which is a generalization of the original Peierls–Nabarro model [26] using the Galerkin finite element scheme [27]. This model allows multiple glide planes to be considered simultaneously for core spreading. Hence potentially complex cores, such as non-collinear partial Burgers vectors or cores spreading simultaneously in several planes, can be modeled [28,29]. We use *Cod*^{2}*ex*, a code implemented by Denoual and co-workers [11,12,30] which describes a dislocation core as resulting from the balance between elastic and interaction force in order to minimize the total energy ε of the system. For the sake of clarity (for a precise description, the reader may refer to Ref. [12]), in the case of single γ-surface energy, the total energy of the system can be written as:

$$\varepsilon = \int_v \left\{ E^e[u,f] - \frac{1}{2}\Omega \ddot{u}^2 \right\} dV + \int_\Sigma E^{isf}[f] d\Sigma$$

where Ω corresponds to the material density, E^e corresponds to the elastic strain energy and E^{isf} is the inelastic stacking fault energy, a function of γ-surface energy without the linear elastic part controlling the spreading of dislocation. The field f follows a time-dependent Ginzburg–Landau equation, considering an element-free