



Full length article

# Multiscale description of carbon-supersaturated ferrite in severely drawn pearlitic wires



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## ABSTRACT

A multiscale simulation approach based on atomistic calculations and a discrete diffusion model is developed and applied to carbon-supersaturated ferrite, as experimentally observed in severely deformed pearlitic steel. We employ the embedded atom method and the nudged elastic band technique to determine the energetic profile of a carbon atom around a screw dislocation in bcc iron. The results clearly indicate a special region in the proximity of the dislocation core where C atoms are strongly bound, but where they can nevertheless diffuse easily due to low barriers. Our analysis suggests that the previously proposed pipe mechanism for the case of a screw dislocation is unlikely. Instead, our atomistic as well as the diffusion model results support the so-called drag mechanism, by which a mobile screw dislocation is able to transport C atoms along its glide plane. Combining the C-dislocation interaction energies with density-functional-theory calculations of the strain dependent C formation energy allows us to investigate the C supersaturation of the ferrite phase under wire drawing conditions. Corresponding results for local and total C concentrations agree well with previous atom probe tomography measurements indicating that a significant contribution to the supersaturation during wire drawing is due to dislocations.

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## 1. Introduction

Mechanical properties of steels are strongly influenced by interactions between solute atoms, in particular large interstitials such as C, and dislocations [1,2]. The extended strain field of a dislocation provides C atoms with a driving force to redistribute and to concentrate inside the dislocation core [3,4]. The segregation of C atoms to a dislocation forms a cloud—known as Cottrell atmosphere [2,4]—pinning the dislocation and altering its distortion field. To unpin the dislocation from the Cottrell atmosphere an additional force is required. The pinning/unpinning process results in a change of the mechanical properties of steels. If this change takes place after deformation, it is commonly termed *static strain-aging*. If the change in mechanical properties occurs during the plastic deformation, it is called *dynamic aging* and it constitutes a serious hindrance to the manufacture of steels [1]. Besides controlling the mechanical properties, the presence and activity of dislocations also influences the thermodynamic stability of interstitial atoms and consequently changes the local composition of

phases within steels. While the effect of the C-dislocation interaction on the mechanical properties of steels has been the subject of numerous theoretical and experimental studies [1,2,4–8], the effect on the chemical rearrangement of C within the microstructure of steels has attracted less attention.

A steel with great technological importance that critically depends on C-dislocation interactions are severely deformed pearlitic wires with up to 7 GPa strength [9]. Experimental observations have revealed an exponentially increasing density of dislocations [10–12] and a decomposition of the cementite phase [3,13–21] during the severe plastic deformation. The original stoichiometric C-concentration of 25 at.% in cementite substantially decreases (sometimes even to levels of 10 at.%) and the C atoms redistribute within the ferrite (bcc or  $\alpha$ -Fe) lamellae [22]. This redistribution results in a dramatically increased C concentration in the ferrite matrix [3] which is nine orders of magnitude above conventional phase diagram predictions [23]. Several authors [17,24,25] have suggested that there is a correlation between C-dislocation binding energy and the decomposition of cementite. In particular, it has been assumed [3,10] that the C excess atoms from the cementite decomposition are accommodated in the vicinity of dislocations in bcc iron, but so far a quantitative analysis has been lacking. In this

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study, we therefore present a quantitative multiscale investigation of the role of C-dislocation interactions on the experimentally observed ferrite supersaturation in severely deformed pearlitic microstructures.

The accumulation of C in ferrite is generally assumed to be enhanced by kinetic processes during the severe plastic deformation, in particular due to a dislocation-driven transfer of C atoms from the cementite/ferrite interface into the ferritic layers [3,10,13,25]. Two main dislocation-based scenarios for transporting C atoms from ferrite–cementite interfaces into the ferrite region have been proposed:

- **Pipe diffusion mechanism:** Sauvage et al. [25] have proposed that dislocations located in the ferrite phase and/or crossing the ferrite–cementite interface act as accelerated paths (i.e., pipes) for C diffusion from cementite to the trap sites (e.g., grain boundaries) in ferrite. This idea is based on the assumption that the C migration energy profile is disturbed in the vicinity of a dislocation due to core reconstructions resulting in modified C diffusion barriers. In particular, it is believed [26,27] that diffusion in the core region of dislocations where atoms have a different coordination should be faster than in the bulk region.
- **Drag mechanism:** Li et al. [3,22] have suggested that dislocations propagating from the ferrite–cementite interface into the ferrite phase (either by bulging or by the Frank-Read mechanism) can collect C atoms from cementite and drag them into ferrite. For this drag mechanism to apply, it is necessary that two kinetic phenomena—the diffusion of C atoms and the motion of dislocations—occur with rates in the same order of magnitude. Therefore this mechanism is probable either at sufficiently high temperatures, when C diffusion is fast, and/or at relatively low strain rates, when the dislocation velocity is low [8].

Both mechanisms critically depend on the mobility of the C atoms in the vicinity of dislocations. In this work, computer simulations are used to investigate the effect of the dislocation strain field on the stability and mobility of C.

To study these mechanisms requires simulation techniques that capture C diffusion events and also the motion of dislocations in agreement with experiments. The drag of C atoms by dislocations has been previously studied using molecular dynamics simulations [8]. However, since the molecular-dynamics modeling technique is presently not capable to simulate the time scales for realistic strain rates, typical simulations are performed at strain rates much greater than the ones applied in experiments and at rather high temperatures to accelerate C diffusion. In the present study, a multiscale simulation approach—based on atomistic simulations and a discrete diffusion method—is used to overcome the typical limitations of molecular dynamics simulations and thus to study possible dislocation-based mechanisms involved in the decomposition of cementite under realistic conditions.

In our multiscale modeling approach, the information about C stability and mobility in the vicinity of a dislocation is obtained from atomistic simulations and is transferred as input to a diffusion equation. This allows to overcome the time and length scale limitations of atomistic simulations yet preserving the relevant atomistic information when predicting the target quantities. In particular, we calculate C-dislocation interactions using an embedded atom method (EAM) potential and we use the nudged elastic band (NEB) technique in conjunction with the EAM potential to calculate the migration behavior of C in the vicinity of a screw dislocation. In a final step, we use the atomistic information to study the C transport in the core of a moving screw dislocation by solving the discrete diffusion equation in the vicinity of the dislocation.

## 2. Methodology

### 2.1. C-dislocation interaction

The Fe–C EAM potential used in the present work has been developed by Becquart et al. [28]. This binary EAM potential is based on the Fe EAM potential introduced by Mendeleev et al. [29] which has been designed with a special focus on properly describing interatomic interactions at small distances. A consequence is a compact core structure of the screw dislocation in bcc iron in good agreement with *ab initio* calculations [28–30] and the correct description of the octahedral (Oh) site as the most stable interstitial position for C in agreement with experimental observations [31]. C diffusion in  $\alpha$ -Fe and the tetragonality induced by adding C are also in good agreement with experimental data [28].

Carbon atoms can occupy three different types of Oh interstices in bcc iron. Among the six iron atoms forming an Oh interstitial site, the nearest neighbor iron atoms to the center of the interstice are lying along one of the principle axes of the bcc lattice ([100], [010], and [001] direction) and the remaining four iron atoms are lying on the {110} planes. Inserting a C atom into one of the Oh sites induces a strong tetragonality along the direction of the nearest-neighbor iron atoms, limiting the C solubility in ferrite. In the following, Oh sites will be differentiated based on the direction of the nearest-neighbor Fe atoms, i.e., the Oh site which has nearest neighbors along [100] is called  $Oh_{[100]}$ .

Previously we have shown [32] that the presence of an external tensile field dramatically changes the stability of C in an Oh site. Likewise, the strain field of a dislocation changes the stability of C in an Oh site. In order to investigate this effect, we use the following definition for the C-dislocation binding energy:

$$E_{\text{bind}} = E_{\text{dislo+C}} - E_{\text{dislo}} - \mu_{\text{C}}^{\alpha}, \quad (1)$$

where  $E_{\text{dislo+C}}$  is the total energy of a system including both a straight dislocation and a C atom in one of the Oh sites,  $E_{\text{dislo}}$  is the total energy of the system with only a straight dislocation,  $\mu_{\text{C}}^{\alpha}$  is the chemical potential of C taken to be

$$\mu_{\text{C}}^{\alpha} = E_{\alpha\text{Fe+C}} - E_{\alpha\text{Fe}}, \quad (2)$$

with  $E_{\alpha\text{Fe+C}}$  the total energy of bulk Fe with a C interstitial in an Oh site and with  $E_{\alpha\text{Fe}}$  the total energy of a perfect bcc Fe lattice. Based on the definition in Eq. (1), a positive binding energy indicates that the two defects, C and the dislocation, repel each other, and a negative one indicates that they attract each other. As an extension to Eq. (1), we will also compute

$$E_{\text{bind}}(\epsilon_{\text{el}}) = E_{\text{dislo+C}}(\epsilon_{\text{el}}) - E_{\text{dislo}}(\epsilon_{\text{el}}) - \mu_{\text{C}}^{\alpha}, \quad (3)$$

in order to investigate the impact of an externally applied elastic strain,  $\epsilon_{\text{el}}$ , corresponding to a uni-axial strain along the [100] direction for a C atom being placed in one of the  $Oh_{[100]}$  sites.

In all simulations, a screw dislocation is introduced in the center of a simulation box with dimensions of  $145 \times 139 \times 7.4 \text{ \AA}^3$  by displacing atoms according to the anisotropic elasticity description of a line defect in crystalline materials. In particular, the analytical expression developed by Hirth et al. [33] is used for implementing the dislocation into the supercell. During the following atomic relaxation (performed within the LAMMPS code [34]), an outer layer of  $\approx 10 \text{ \AA}$  thickness in all directions perpendicular to the dislocation line is kept fixed to reproduce the extended strain field of the dislocation as obtained from linear elasticity theory. The boundary conditions along the dislocation line for all simulations

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