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Ferrite, martensite and supercritical iron: A coherent elastochemical theory of stress-induced carbon ordering in steel

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ABSTRACT

A mean-field model based on the elasticity theory of point defects has been developed to investigate the role of uniform stress fields on the long-range ordering of carbon atoms in bcc-iron. From an analysis of the thermodynamic equilibria, composition – temperature – stress state diagrams are derived. We demonstrate that ferrite, martensite and *supercritical iron* are various instances of the same bcc-iron phase region. A coherent mapping of the phase transitions is drawn, identifying (i) continuous transitions such as ferrite ordering, martensite enhanced ordering and ferrite – martensite transformation, and (ii) discontinuous transitions such as temperature-induced martensite and stress-induced martensite. Our analysis is supported by rigid-lattice Monte Carlo simulations. Recently published experimental results on highly-drawn perlitic wires are re-interpreted in terms of supercritical iron, rather than strain-induced martensite. Novel low-temperature thermomechanical treatments of supersaturated ferrite are suggested, for improved nanostructure design of martensitic steels.

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1. Introduction

Martensite is a microstructural component that contributes to the hardness of numerous types of high-strength steels, *e.g.* Refs. [1,2]. Its hierarchical microstructure is composition-dependent and comprises packets, blocks, laths and nanotwins [3]. The ultimate structural components are the orientational variants, consisting each of a monocrystalline domain of body-centered tetragonal structure. In a variant, the carbon atoms sit preferentially in one of the three octahedral interstitial sublattices of the reference bcc structure. The resultant tetragonal distortion of the crystal gives rise to the bct structure, with an axial c/a ratio greater than one. The crystals of martensite are subjected to internal stresses of all orders, which may amount to the gigapascal [4]. Carbon supersaturation is also a major characteristic of martensite crystals. In usual situations, the spatial distribution of carbon is inhomogeneous at various scales, due to autotempering and segregation on structural defects [5,6]. There exist specific experiments where the carbon content has been measured locally: in subzero- M_s alloys [7] and in heavily-drawn wires [8]. These experiments allow for a direct quantification of the effect of solute carbon on lattice tetragonality.

The occurrence of tetragonality in martensite may be viewed as a consequence of the austenite to martensite displacive transformation during quench, following the Bain mechanism [9]. Alternatively, it has been described as the result of long-range ordering of the carbon atoms during cooling after the transformation of austenite [10]. Zener [11] developed a mean-field model describing the degree of order and the resultant tetragonal deformation of a supersaturated Fe-C alloy, as function of composition and temperature. According to Zener, the driving force for carbon ordering is the strain interaction between each carbon atom and the elastic strain induced by the other carbon atoms. Recent works [12,13] have proven that elasticity is indeed the major source of the driving force for ordering and disordering in this system. At equilibrium, the ordering is only partial since the configurational entropy tends to redistribute the carbon atoms randomly onto the three octahedral sublattices. The balance between energy and entropy results in the existence of an order-disorder transition between ferrite and martensite. By a mean-field approach, Khachatryan et al. [14] showed that the order-disorder transition is of first order, and provided an analytical formula for the transition temperature in a stress-free Fe-C alloy. This type of model succeeded in predicting the degree of order as function of temperature, and the occurrence of temperature hysteresis [13]. Various works provided refinements on the prediction of the order-disorder transition and its effect on the lattice parameters of bct-

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iron, e.g. Refs. [15–18]. Khachatryan et al. [14] also showed that, in alloys containing residual austenite, the internal coherency stresses modify the level of carbon ordering in martensite, and produce a continuous variation of order with temperature, accompanied with an “ordering tail” at high temperature.

Recently, Mirzaev et al. [19,20] proposed various mean-field models of carbon ordering under applied stress that deny the existence of the ordering tail. From molecular dynamics simulations, they conclude that an ordering tail can be the result of short-range interactions [21]. In recent works, Nematollahi, Djaziri et al. [8,22] claimed the occurrence of strain-induced martensite in isothermally deformed supersaturated bcc-iron of heavily-drawn perlite steels. They developed a mean-field model from which the asserted mechanism of ferrite to martensite transformation is the ordering of carbon atoms when the strain exceeds a threshold value. However, they did not explain quantitatively the magnitudes of the tetragonal distortion that they measured, neither the fact that the measured c/a ratio appears continuous as function of solute carbon content.

In this context, it appears that clarification of the mechanisms of isothermal carbon ordering in bcc-iron is needed. One has to recognize first that, albeit specific cases (atom probe needle tip or nanosize monocrystalline beam), bulk stress-free Fe-C crystals can never be encountered in practice. From the crystallographic point of view, a crystal of bcc-ferrite deformed along one of its axes loses its cubic symmetry and acquires the tetragonal symmetry: it becomes isostructural to bct-martensite. In this view, deformed ferrite and martensite pertain to the same phase region [23]. This suggests the possibility of a continuous transformation from ferrite to martensite, and reversely. Second, as a consequence of internal or external stresses, ferrite itself is never fully disordered. This is evidenced by internal friction experiments, where the Snoek peak [24] is the result of alternative carbon ordering from one interstitial sublattice to another, as the strain is reversed. This phenomenon is known to occur in low carbon steels, although not in martensite [25]. On the modelling side, Garruchet et al. [26] computed a Snoek peak by straining a bcc-Fe crystal in a molecular dynamics simulation: the crystal cell alternates from prolate tetragonal to oblate tetragonal as the stress turns from tensile to compressive along the cell axis.

The literature review above suggests that ferrite and martensite¹ are instances of the same phase, and are both subject to carbon ordering. Following Landau [27], we thus expect that the stress – temperature phase diagram at constant carbon composition will include (i) a first-order transition line between ferrite and martensite, and (ii) a critical point around which the ferrite ↔ martensite transition is continuous.

In order to rationalize the above-mentioned facts, a coherent theory of stress-induced carbon ordering is needed. It should incorporate the effect of stresses on the relative stability of ferrite and martensite. Such a theory is of practical importance since prediction of the order-disorder transition temperature is a prerequisite to controlling the microstructure and properties of martensite after quench or after low-temperature ageing [7]. Furthermore, understanding the role of solute carbon is essential to alloy optimization of dual phase [28], quenched and partitioned [2], and bainitic steels [29].

In this paper, we focus on the ordering behavior of carbon in a supersaturated bct-Fe crystal isothermally transformed under fixed

stress and uniform composition. Following Zener and Khachatryan, we rely on the mean-field approximation of uniform carbon-induced strain, and we make use of the elasticity theory of point defects [30–32]. We build the functional form of the elastochemical Gibbs energy, from which stress – temperature and composition – temperature phase diagrams are constructed. Analytical equations are derived as far as possible and are solved numerically when necessary. The validity of our analysis is tested by comparison with rigid-lattice Monte Carlo simulations. The existence of a critical line in the phase diagram is demonstrated, and the concept of supercritical bct-iron is introduced. The temperature and stress hysteresis phenomena are highlighted. Conditions for the occurrence of stress-induced martensite, for martensite enhanced ordering, and for continuous ferrite – martensite transition are discussed. In the light of our theory, the experimental results of Nematollahi et al. are re-interpreted and compared to our calculations.

2. Elastochemical mean-field model

Our elastochemical model aims at predicting the distribution of carbon atoms over the sublattices of a Fe-C crystal variant as function of composition, temperature and applied stress. The thermodynamics of a system under applied stress is driven by the generalized Gibbs energy, which is the state function to be extremal at equilibrium. In this section, we start from the analytical form of the enthalpy and entropy functions and apply the mechanical and chemical equilibrium conditions to derive the equation of internal equilibrium of the Fe-C solid solution. The conditions for stability of the various carbon distributions will be further discussed.

From elasticity theory [30–32], the elastic part of the energy of a crystal of volume \mathcal{V} containing a population of point defects, and submitted to an applied homogeneous strain is, per iron atom

$$E = \frac{1}{2}V_0\mathbf{C}\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} - \mathbf{P} : \boldsymbol{\varepsilon}. \quad (1)$$

In this equation, $V_0 = \frac{1}{2}a_0^3$ is the volume per iron atom of unstrained ferrite, \mathbf{C} is the stiffness tensor, $\boldsymbol{\varepsilon}$ is the strain tensor, \mathbf{P} is the elastic dipole tensor of the defects (per iron atom). The first term is the lattice strain energy; the second is the solute-strain interaction energy, which depends on the carbon distribution via the components of \mathbf{P} . Under applied stress $\boldsymbol{\sigma}$, one has to consider the generalized enthalpy, derived from the energy by a Legendre transformation [33]:

$$H = \frac{1}{2}V_0\mathbf{C}\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} - \mathbf{P} : \boldsymbol{\varepsilon} - V_0\boldsymbol{\sigma} : \boldsymbol{\varepsilon}. \quad (2)$$

The reference state for H is the unstrained cubic ferrite of atomic volume V_0 . One can check that under isostatic pressure p , the generalized enthalpy reduces to its expected form $H = E + p(V - V_0)$, where V is the actual atomic volume. The composition dependence of the stiffness \mathbf{C} can be neglected, since the C_{ij} 's vary by less than 1% per at.% of carbon [34,35]. Mechanical equilibration being much faster than chemical equilibration, the condition for mechanical equilibrium holds at any time during carbon redistribution. Hence, the mechanical equilibrium condition can be treated independently, considering \mathbf{P} has a constant. Under the applied stress $\boldsymbol{\sigma}$ and given the dipole tensor \mathbf{P} , mechanical equilibrium is realized for a strain $\boldsymbol{\varepsilon}^{\text{eq}}$ corresponding to the extremum of $H(\boldsymbol{\varepsilon})$:

$$\boldsymbol{\varepsilon}^{\text{eq}} = \mathbf{S} \left(\boldsymbol{\sigma} + \frac{\mathbf{P}}{V_0} \right), \quad (3)$$

¹ In this paper, “ferrite” and “martensite” are in contrast to the standard definitions in steel physical metallurgy books: we generalized the term “ferrite” to low-order low-tetragonality crystals of bct-iron. We called “martensite” the crystal variants of high-order high-tetragonality bct-iron. These definitions reduce to usual ferritic (bcc) and martensitic (bct) crystal structures when the stress tends to zero.

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