Journal of Nuclear Materials 386–388 (2009) 45–48

Contents lists available at ScienceDirect

Journal of Nuclear Materials

journal homepage: www.elsevier.com/locate/jnucmat

The magnetic origin of anomalous high-temperature stability of dislocation loops in iron and iron-based alloys

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A B S T R A C T

The dominant occurrence of the $\mathbf{b} = a\langle 001\rangle$ prismatic edge dislocation loops in iron and iron-based alloys irradiated at temperatures approaching 500 °C is a striking anomaly distinguishing iron and its alloys from other bcc metals. It is surprising that the $a\langle 001\rangle$ dislocation loops form at all, since there is an alternative $\mathbf{b} = a/2\langle 111\rangle$ dislocation loop configuration that, according to the conventional isotropic treatment of elasticity, has a lower self-energy. In this paper we highlight the magnetic aspect of the problem and note the fundamental link between the α–γ phase transition, the elastic anisotropy of iron, which is particularly significant at elevated temperatures, and thermal magnetic fluctuations.

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1. Introduction

The frequent occurrence of the $\mathbf{b} = a\langle 001\rangle$ prismatic edge dislocation loops in bcc iron and iron-based alloys irradiated at high temperatures is one of the most surprising phenomena in the field of radiation damage of materials [1–4]. It is very unusual that the $a\langle 001\rangle$ loops form at all, since there is an alternative $\mathbf{b} = a/2\langle 111\rangle$ loop configuration that, according to the conventional isotropic treatment of elasticity, has a lower self-energy.

In this paper, we argue that this high-temperature radiation damage anomaly has magnetic origin.

Magnetism has important implications for the structural stability of iron-based alloys and steels. The equilibrium structure of atomic configurations depends sensitively on magnetic ordering in the case where the magnetic energy and the difference between energies of competing crystal structures are comparable. Hasegawa and Pettifor [5] showed that magnetism stabilizes the body-centred cubic (bcc) α-phase of iron at low temperatures. This assertion is supported by density functional calculations [6] showing that the energy per atom in the non-magnetic or in the antiferromagnetic bcc phases of iron is higher than the energy of any of the fcc phases. Thermal magnetic fluctuations are responsible for the phase transition from the bcc α to the fcc γ phase occurring approximately at 912 °C.

As a precursor for this structural phase transformation, iron and iron-based alloys exhibit gradual softening of the stiffness constant $c' = (c_{11} - c_{12})/2$ that, according to experimental measurements [7,8], decreases by a factor of three between the room temperature and 800 °C. Such a strong variation of c' affects the energy of interaction between dislocations, as well as the self-energies of dislocation loops in iron and iron-based alloys. This has a profound effect on the mechanical properties [9]. The strong temperature dependence of stiffness constants of iron looks particularly striking in comparison with the case of non-magnetic bcc metals, where no significant variation of stiffness constants is observed over the same interval of temperatures [10].

The effect of softening of c' in the vicinity of the α–γ phase transition cannot *in principle* be described using the 'conventional' isotropic treatment of elasticity, where the elastic properties are characterized by only *two* independent parameters, such as the shear and the bulk moduli, or the Young modulus E and the Poisson ratio σ [11]. To prove this we note that in the isotropic elasticity approximation, for any choice of these two parameters, the spectrum of elastic acoustic waves described by the wave equation

$$\rho \ddot{u}_l = \frac{E}{2(1+\sigma)} \frac{\partial^2}{\partial x_i^2} u_l + \frac{E}{2(1+\sigma)(1-2\sigma)} \frac{\partial^2}{\partial x_l \partial x_i} u_i,$$

where ρ is the mass density of the material, consists of one longitudinal and two transverse modes with group velocities

$$c_l = \left[\frac{E(1-\sigma)}{\rho(1+\sigma)(1-2\sigma)}\right]^{1/2} \qquad (1)$$

and

$$c_t^{(1,2)} = \left[\frac{E}{2\rho(1+\sigma)}\right]^{1/2}.$$

These velocities are independent of the direction of propagation of waves through the lattice, and *none* of them vanishes for *any*

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doi:10.1016/j.jnucmat.2008.12.303

reasonable choice of E and σ. For example, in the isotropic elasticity approximation we do not find the remarkable $\mathbf{k}\|(1\,1\,0)$ $\mathbf{e}\|(1\,\bar{1}\,0)$ phonon mode [12] that softens near the α–γ phase transition temperature, providing the pathway for the bcc/fcc structural transformation. This argument shows that the isotropic elasticity approximation is not suitable for modelling iron and iron-based alloys anywhere in the vicinity of the α–γ phase transition temperature.

Now we present an argument suggesting that magnetic fluctuations may explain the strong variation of stiffness parameters of iron as a function of temperature, and discuss the implication of the observed elastic softening of iron for the relative stability of dislocation loops. Starting from a tight-binding Hamiltonian formalism that includes *only* the on-site Coulomb interactions, we derive a many-body Stoner Hamiltonian originally postulated in Ref. [12], and develop a qualitative argument showing that strong temperature dependence of forces acting between atoms can emerge on the timescale comparable to the timescale of atomic vibrations. We conclude by assessing the effect of elastic softening on the free self-energies of dislocations and dislocation loops [4] and show that this explains the observed occurrence of the $\mathbf{b} = a\langle 0\,0\,1\rangle$ dislocation loops in iron and iron-based alloys at elevated temperatures.

2. The magnetic tight-binding Hamiltonian

In the tight-binding approximation the many-body quantum Hamiltonian for d-electrons in a transition metal has the form [13,14]

$$\begin{aligned}\hat{H} = &\sum_{i,j,i\neq j}\sum_{m,m',\sigma} t_{im,jm'}\hat{c}^{\dagger}_{im\sigma}\hat{c}_{jm'\sigma} + \sum_{i,m,\sigma}\epsilon_i\hat{c}^{\dagger}_{im\sigma}\hat{c}_{im\sigma}\\ &+\left[\frac{\bar{U}}{2}\sum_{i}\sum_{m,m',\sigma}\hat{n}_{im,\sigma}\hat{n}_{im',-\sigma}\right.\\ &\left.+\frac{(\bar{U}-\bar{J})}{2}\sum_{i}\sum_{m,m',\sigma}\hat{n}_{im,\sigma}\hat{n}_{im',\sigma}(1-\delta_{mm'})\right]+\hat{H}'. \end{aligned} \qquad (2)$$

Here the t-term is the operator of kinetic energy of electrons associated with hopping between d-orbitals situated on sites i and j, ϵ_i is the single-particle on-site energy, and the third and fourth terms represent interaction between electrons. $\hat{H}'$ completes the Hamiltonian by adding the contribution of the nearly-free-electron s–p band. This latter term plays a significant part only at short distances between atoms.

Hamiltonian (2) contains several terms describing interatomic interactions in a transition metal. The first is related to the formation of chemical bonds due to the hybridization of atomic d-orbitals. These bonds are described by the t-terms in (2). A hopping (hybridization) matrix element $t_{im,jm'}$ involves an orbital m centered on site i, and an orbital m' centered on site j.

A term in Hamiltonian (2), which until recently received no attention in connection with the semi-empirical treatment of interatomic interactions, is the term describing electron-electron interactions and magnetism. It is well known that the Hubbard U-term suppresses hopping of electrons and hence weakens chemical bonding in a material [15]. This was also noted in connection with the treatment of interatomic cohesion in the LSDA+U model [14]. The on-site interaction between electrons is described by the term in square brackets in (2). Parameter $\bar{U}$ is the Coulomb energy of repulsion between a pair of electrons with antiparallel spins occupying the same lattice site, and $\bar{J}$ characterizes the strength of *intra-atomic* exchange between electrons. The on-site interaction part of the Hamiltonian can also be written as

$$\begin{aligned}\hat{H}_i = &\bar{U}\sum_{m,m'}\hat{n}_{im\uparrow}\hat{n}_{im'\downarrow}\\ &+\frac{(\bar{U}-\bar{J})}{2}\sum_{m,m',m\neq m'}[\hat{n}_{im\uparrow}\hat{n}_{im'\uparrow}+\hat{n}_{im\downarrow}\hat{n}_{im'\downarrow}].\end{aligned} \qquad (3)$$

The second term in (3) vanishes completely for the case of s-electrons (or, in other words, in the case of a single band Hubbard model). In this case there is only one tight-binding orbital per lattice site, $m = m' = 0$, and no possibility remains for the intra-atomic Coulombic exchange interaction.

Hamiltonian (3) can be simplified further by introducing the operator of the total number of electrons occupying a lattice site $\hat{N}_i = \hat{N}_{i\uparrow} + \hat{N}_{i\downarrow}$ and the operator of the total magnetic moment $\hat{M}_i = \hat{N}_{i\uparrow} - \hat{N}_{i\downarrow}$. Using these operator notations, we simplify (3) as [16]

$$\hat{H}_i = \frac{\bar{U}}{2}(\hat{N}_i^2 - \hat{N}_i) - \frac{\bar{J}}{4}(\hat{N}_i^2 - 2\hat{N}_i) - \frac{\bar{J}}{4}\hat{M}_i^2. \qquad (4)$$

There are two types of terms in this Hamiltonian. The terms that depend on $\hat{N}_i$ describe fluctuations of energy due to fluctuations of the total number of electrons on a given lattice site. On the other hand, the term $-\bar{J}\hat{M}_i^2/4$ lowers the energy by forming a non-zero magnetic moment on the site, in accord with Hund's rule. If we neglect fluctuations of the total number of electrons on a site (in which case the expectation value of $\hat{N}_i$ is kept constant for example by the charge neutrality condition) and appropriately adjust the on-site energies ϵ_i to satisfy this condition, we arrive at the Stoner Hamiltonian [12]

$$\hat{H}_{Stoner} = \sum_{i,j,i\neq j}\sum_{m,m',\sigma} t_{im,jm'}\hat{c}^{\dagger}_{im\sigma}\hat{c}_{jm'\sigma} + \sum_{i,m,\sigma}\epsilon_i\hat{c}^{\dagger}_{im\sigma}\hat{c}_{im\sigma} - \frac{I}{4}\sum_i \hat{M}_i^2, \qquad (5)$$

where we identified $\bar{J}$ with the Stoner parameter I. Due to the operator form of the magnetic Stoner term, this Hamiltonian is expected to be of similar complexity to the Hubbard Hamiltonian [17]. At the same time the physical picture described by the Stoner Hamiltonian (5) is completely different to that of the Hubbard Hamiltonian. The derivation given above shows that the Stoner parameter I in Eq. (5) describes intra-atomic exchange. This term bears no relation to the direct Coulomb interaction between electrons described by the U-term in a simple s-band-type Hubbard model [17].

3. The temperature-dependent interatomic forces

What is the functional form of the expectation value of Stoner Hamiltonian (5)? Consider a trial wave function Ψ describing an electronic configuration for an arbitrary set of coordinates of atoms $\mathbf{R}_1, \ldots, \mathbf{R}_N$, and a corresponding set of expectation values of local magnetic moments $\mathbf{M}_1, \ldots, \mathbf{M}_N$. The Stoner Hamiltonian (5) is quadratic in $\hat{M}_i$ and is invariant with respect to the rotation of the direction of quantization of magnetic moments. Hence the expectation value of energy $\langle\Psi|\hat{H}_{Stoner}|\Psi\rangle$ also has to be invariant with respect to the choice of direction of this axis. A sufficiently general form of a function of coordinates of atoms and magnetic moments that satisfies this condition is

$$\begin{aligned}E(\mathbf{R}_1,\ldots,\mathbf{R}_N;\mathbf{M}_1,\ldots,\mathbf{M}_N) &= \langle\Psi|\hat{H}_{Stoner}|\Psi\rangle\\ &= E^{(0)}(\mathbf{R}_1,\ldots,\mathbf{R}_N)\\ &\quad+\sum_i E_i^{(1)}(\mathbf{R}_1,\ldots,\mathbf{R}_N)\mathbf{M}_i^2\\ &\quad+\sum_i E_i^{(2)}(\mathbf{R}_1,\ldots,\mathbf{R}_N)(\mathbf{M}_i^2)^2\\ &\quad+\sum_{i,j,i\neq j} E_{ij}^{(3)}(\mathbf{R}_1,\ldots,\mathbf{R}_N)\mathbf{M}_i\cdot\mathbf{M}_j+\ldots\end{aligned} \qquad (6)$$

This expansion contains an infinite number of terms involving even powers of magnetic moments, as well as scalar products of moments associated with different lattice sites.

By minimizing the energy $E(\mathbf{R}_1,\ldots,\mathbf{R}_N;\mathbf{M}_1,\ldots,\mathbf{M}_N)$ with respect to the *magnitude* of magnetic moments $|\mathbf{M}_1|,|\mathbf{M}_2|,\ldots,|\mathbf{M}_N|$ (this minimization only requires redistributing electrons between the spin states within each atom, and it does not interfere with the local charge neutrality condition), we arrive at a general formula for the energy of a system of atoms, which is invariant with respect to the choice of the direction of quantization axis for magnetic moments, and is characterized by the positions of atoms $\mathbf{R}_1,\ldots,\mathbf{R}_N$ and the directions of unit vectors of magnetic moments $\mathbf{e}_1,\ldots,\mathbf{e}_N$, namely

$$\begin{aligned} &E(\mathbf{R}_1,\ldots,\mathbf{R}_N;\mathbf{e}_1,\ldots,\mathbf{e}_N) \\ &\quad = U(\mathbf{R}_1,\ldots,\mathbf{R}_N) - \frac{1}{2}\sum_{i\neq j} J_{ij}(\mathbf{R}_1,\ldots,\mathbf{R}_N)\mathbf{e}_i\cdot\mathbf{e}_j + \ldots \end{aligned} \tag{7}$$

Functions $U(\mathbf{R}_1,\ldots,\mathbf{R}_N)$ and $J_{ij}(\mathbf{R}_1,\ldots,\mathbf{R}_N)$ depend on the positions of atoms and parameters of the Stoner Hamiltonian (5). In principle they can be evaluated using a suitable approximation for the trial wave function Ψ, or the Green's functions formalism. In a ferromagnetic configuration, where all the moments are parallel to each other, and where $\mathbf{e}_i\cdot\mathbf{e}_j = 1$ for all i and j, energy (7) depends only on coordinates of atoms, and is subject to a constraint that the magnitude of each magnetic moment is determined by the condition that the total energy (6) is minimum. This limiting case of a ferromagnetically ordered (but geometrically arbitrarily distorted) atomic configuration was investigated in Refs. [18,19] and led to the development of a 'magnetic' interatomic potential.

In principle, both coordinates of atoms and the directions of magnetic moments can be treated as dynamical variables [20,21]. We will not discuss this here and instead consider, in qualitative terms, the effect of thermal fluctuations of magnetic moments on the forces acting between atoms in a magnetic transition metal. Replacing the product $\mathbf{e}_i\cdot\mathbf{e}_j$ by the correlation function of directions of magnetic moments

$$\xi_{ij}(\mathbf{R}_1,\ldots,\mathbf{R}_N,T) = \langle \mathbf{e}_i\cdot\mathbf{e}_j\rangle_T = \lim_{t\to\infty}\frac{1}{t}\int_0^t \mathbf{e}_i(t')\cdot\mathbf{e}_j(t')dt', \tag{8}$$

we find the average force acting on atom k

$$\begin{aligned} \mathbf{F}_k = &-\frac{\partial}{\partial\mathbf{R}_k}U(\mathbf{R}_1,\ldots,\mathbf{R}_N) \\ &+\frac{1}{2}\frac{\partial}{\partial\mathbf{R}_k}\sum_{i\neq j}J_{ij}(\mathbf{R}_1,\ldots,\mathbf{R}_N)\xi_{ij}(\mathbf{R}_1,\ldots,\mathbf{R}_N,T). \end{aligned} \tag{9}$$

This equation illustrates the fundamental difference between forces acting between atoms in a magnetic and in a non-magnetic metal. Eq. (9) shows that forces acting between 'magnetic' atoms *explicitly* depend on temperature due to the temperature dependence of the correlation function of magnetic moments $\xi_{ij}(\mathbf{R}_1,\ldots,\mathbf{R}_N,T) = \langle\mathbf{e}_i\cdot\mathbf{e}_j\rangle_T$. The directions of magnetic moments fluctuate and hence forces acting between the atoms in a magnetic metal for the same set of coordinates $\mathbf{R}_1,\ldots,\mathbf{R}_N$ are not the same for any two different temperatures of the spin subsystem [20,21]. The higher-order derivatives of the total energy, like stiffness constants, should also be expected to exhibit unusual dependence on temperature in comparison with the non-magnetic case, where the temperature dependence of interatomic forces originates from the non-harmonicity of interatomic potentials [22]. It is such a dependence that should explain the fairly strong variation of stiffness constants with temperature observed experimentally [7,8].

4. The temperature-dependent self-energies of dislocations

To provide an example illustrating the effect of variation of stiffness constants as a function of temperature on properties of materials, we consider the effect of this temperature variation on the elastic free self-energies of dislocations in bcc iron. In the anisotropic treatment of elasticity, the pre-logarithmic free energy factor of a straight dislocation with Burgers vector $\mathbf{b}$ and the tangent vector $\mathbf{t}$ in an infinite anisotropic medium is [23]

$$\widehat{F}(\mathbf{t}) = \frac{1}{2\pi} b_i b_m n_j n_q c_{ijkl} c_{npmq} \Im\left[\sum_{\kappa=1}^{3} \kappa_p^\eta \kappa_l^\eta \frac{N_{kn}(\boldsymbol{\kappa}^\eta)}{n_s \frac{\partial D(\boldsymbol{\kappa}^\eta)}{\partial \kappa_s}}\right], \tag{10}$$

where for an edge dislocation $\boldsymbol{\kappa}^\eta = \mathbf{m} + \mathbf{n}\omega^{(\eta)}$, $\mathbf{n} = \mathbf{b}/b$, $\mathbf{m} = \mathbf{n}\times\mathbf{t}$, and $\omega^{(1)}$, $\omega^{(2)}$ and $\omega^{(3)}$ are the three complex roots of the sextic equation

$$S(\omega) = \det\left[c_{ijkl}(m_j + n_j\omega)(m_l + n_l\omega)\right] = 0, \tag{11}$$

situated in the upper half of the complex plane $\omega = \Re\omega + i\Im\omega$. $N_{ik}(\boldsymbol{\kappa})$ is a matrix adjoint to $L_{ik}(\boldsymbol{\kappa}) = c_{ijkl}\kappa_j\kappa_l$, and $D(\boldsymbol{\kappa}) = \det L_{ik}(\boldsymbol{\kappa})$. Here c_{ijkl} is the tensor of temperature-dependent stiffness constants that in a crystal of cubic symmetry has 21 non-zero components

$$c_{ijkl} = c_{12}\delta_{ij}\delta_{kl} + c_{44}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + (c_{11} - c_{12} - 2c_{44})\delta_{ij}\delta_{ik}\delta_{il}. \tag{12}$$

The elastic self-energy of an edge dislocation depends on its orientation vector $\mathbf{t}$. Fig. 1 shows the ratio of pre-logarithmic factors evaluated for straight $\mathbf{b} = a\langle 001\rangle$ and $\mathbf{b} = a/2\langle 111\rangle$ edge dislocations plotted as a function of the angle between the direction $\mathbf{t}$ of the dislocation line, and one of the directions where this elastic energy is minimum (these directions are $[100]$ for the $\mathbf{b} = a\langle 001\rangle$ dislocation and $[11\bar{2}]$ for the $\mathbf{b} = a/2\langle 111\rangle$ dislocation). With the exception of tungsten, the curves shown in Fig. 1 systematically deviate from the isotropic elasticity limit, where the ratio of the two energies equals the square of the ratio $\mathbf{b}_{001}^2/\mathbf{b}_{111}^2 = 4/3$. Fig. 1 shows that iron becomes increasingly elastically more anisotropic as temperature approaches the temperature of the bcc–fcc transition T_C =912 °C. We note that experimental values of the elastic constants were used for all materials and temperatures. The curves shown in Fig. 1 also suggest that the elastic self-energy of $a\langle 001\rangle$ edge dislocations decreases faster as a function of temperature than the energy of the $a/2\langle 111\rangle$ dislocations. To investigate this, in Fig. 2 we plotted the

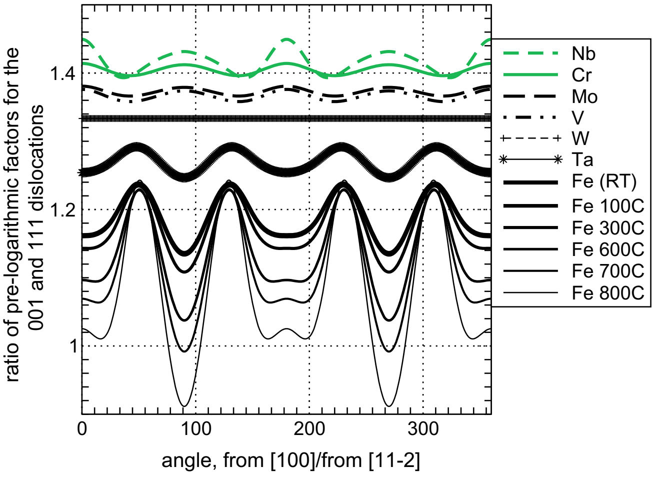

Fig. 1. Ratio of pre-logarithmic factors (10) for straight $\mathbf{b} = a[001]$, $\mathbf{b} = a/2[111]$ edge dislocations evaluated, in the anisotropic elasticity approximation, for several bcc metals as described in the text. In the isotropic elasticity approximation this ratio is independent of the orientation of the tangent vector of the dislocation line and equals 1.3333…. For tungsten, which is nearly elastically isotropic, this ratio is very close to 4/3 = 1.333….

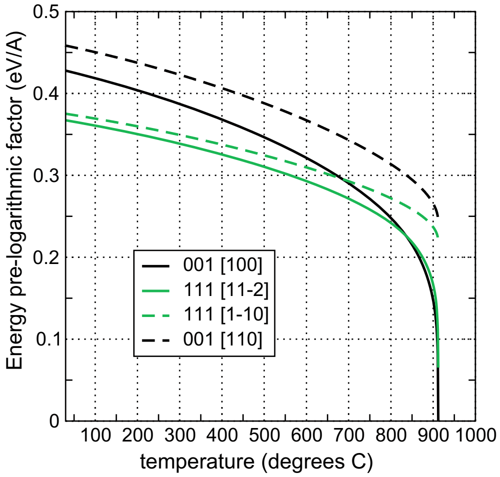

Fig. 2. The leading pre-logarithmic terms (10) in the elastic free energy for straight $\mathbf{b} = (a/2)[1\,1\,1], \mathbf{t} = (1/\sqrt{6})[1\,1\,\bar{2}]$ or $\mathbf{t} = (1/\sqrt{2})[1\,\bar{1}\,0]$, and $\mathbf{b} = [0\,0\,1], \mathbf{t} = [1\,0\,0]$ or $\mathbf{t} = (1/\sqrt{2})[1\,1\,0]$ edge dislocations evaluated as a function of T near the temperature T_C of the α–γ phase transition. The two lowest energy curves intersect approximately at 820 °C. Note that the treatment does not include the contribution of the dislocation core energy terms.

temperature-dependent pre-logarithmic self-energy factors evaluated for the two types of dislocations using values of stiffness constants found by interpolating the experimental values towards the transition temperature T_C. We have taken into account the fact that since the bcc–fcc transformation follows the Bain pathway, the stiffness constant $c' = (c_{11} - c_{12})/2$ is expected to vanish at or near the transition temperature T_C. The curves shown in Fig. 2 suggest that the free self-energy of the $\mathbf{b} = a\langle 1\,0\,0\rangle[0\,0\,1]$ edge dislocation decreases more sharply near the α–γ transition temperature than the free self-energy of the $\mathbf{b} = a/2\langle 1\,1\,1\rangle[1\,1\,\bar{2}]$ edge dislocation. The elastic free self-energies of dislocations with the same Burgers vectors but different line orientations do not exhibit significant temperature variation near T_C. This analysis, as well as the results of a full investigation addressing the dislocation core energy terms as well as the effect of the shape and the size of dislocation loops [4], suggests that the effect of softening of the stiffness constant c' on the elastic free self-energies of dislocations and dislocation loops near the temperature of the α–γ phase transition provides the likely explanation for the observed frequent occurrence of the square-shaped $\mathbf{b} = a\langle 0\,0\,1\rangle$ prismatic dislocation loop configurations at elevated temperatures in bcc iron.

Acknowledgements

The authors gratefully acknowledge stimulating discussions with K. Arakawa, V. V. Bulatov, B. Eyre, A. P. Sutton and C. H. Woo. This work was supported by the UK Engineering and Physical Sciences Research Council and by EURATOM through the Fusion Materials Modelling Programme.

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