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The elasticity of the ½ a_0 <111> and a_0 <100> dislocation loop in α-Fe thin foil

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ABSTRACT

Dislocation loops in irradiated ferritic steels have a Burgers vector of the type ½ a_0 <111> or a_0 <100>. When they are located in a thin foil such as the one used in transmission electron microscopy, the presence of the two free surfaces modify the elastic field by the action of the so-called ‘image forces’, which can in turn influence the loops. In this work, a general analytical method was deployed to calculate the image forces in an anisotropic bcc α-Fe thin foil containing a nanometric dislocation loop. We observe that image forces induce an out of plane displacement that doubles the bulging of the thin foil surfaces induced by the loop. The elastic field and energy induced by the image forces become remarkable when the depth of the dislocation loop is comparable to its size. Moreover, there is large difference in the response to image forces between the ½ a_0 <111> and the a_0 <100> loop, with a stronger one for the ½ a_0 <111> loop, which relates to the anisotropy of the α-Fe.

1. Introduction

Thin foil geometry implies the presence of two free surfaces that impact the elastic field of the foil, which in turn can modify its physical properties relative to the ones of the corresponding infinite medium. This has been recognized at several occasions, for example in the case of the mechanism of the mobility of dislocations in a Cu thin film [1] or a Au thin film [2], which changes with the film thickness. It has been recognized a while ago [3] that irradiation at room temperature of pure α-Fe, representative of ferritic steels, in the form of a transmission electron microscopy (TEM) thin film leads to a majority of a_0 <100> dislocation loops while irradiated Fe in the bulk form exhibits mainly ½ a_0 <111> [3]. This has been attributed to the so-called ‘image forces’ due to the presence of the free surfaces that would attract the mobile ½ a_0 <111> loops to the surfaces, where they disappear. This has been considered in more recent experimental studies in irradiated Fe, by discarding in TEM studies too thin areas (<50 nm) because the proximity of the free surfaces strongly influences the radiation induced microstructure [4], with in addition a significant effect of the specimen crystal orientation on the defect yield [5]. Very recently this has been rationalized by calculation in order to estimate the loop loss in a thin foil due to image forces, using molecular dynamics simulations and isotropic elasticity. It appears that this loss of 5 nm ½ a_0 <111> loops in a 50 nm thin Fe foil amounts to about 30% [6]. However, anisotropy may have a strong impact there as α-Fe has a remarkable anisotropic ratio of 2.4 at room temperature, reaching 7.4 at 900 °C [7]. In terms of elastic formation energy, calculations indicate that the ½ a_0<111> loops at room temperature are more favorable than a_0 <100> loops. With increasing temperature the strong change in anisotropic ratio favors the a_0<100> loops over the ½ a_0 <111> ones, above about 350 °C [8]. This was observed in ferritic steels as well [9]. Nonetheless, as pointed earlier, there are early TEM observations reporting a_0 <100> loops at room temperature, which is confirmed by more recent ones [10–14]. The origin of the observed a_0 <100> loops at room temperature is therefore still unclear; they may result from the interaction of the mobile ½ a_0 <111> loops, as

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proposed earlier [15] and as confirmed more recently by molecular dynamics calculations [16,17], or from the direct transformation of 3D agglomerates of interstitials (such as the C15 cluster [18]) resulting from the displacement cascades, as recently deduced from experiments [11]. In addition, the aforementioned effect of the free surfaces of TEM samples mobilizes the ½ a_0<111> loops along their Burgers vector, which in turn could then either form the a_0<100> loops by mutual interaction or disappear at the surfaces. To clarify the issue, it is therefore critical to properly understand the bias on the radiation induced dislocation loops induced by the use of a thin foil for TEM observations.

In this work, the elastic field induced by a nanometric dislocation loop with either a_0 <100> or ½ a_0 <111> Burgers vector in a thin foil of Fe is studied, taking into account the image forces and the anisotropic character of Fe [19]. The total elastic field, as the displacement or the stress field and their gradient, of the thin film containing the dislocation loop is the sum of the bulk elastic field and the image elastic field. To calculate it, the superposition method we have developed in Fourier space for anisotropic crystals is employed [20]. The elastic energy of the thin film in presence of the dislocation loop is considered and is derived here. More to the point, comparison between the isotropic and anisotropic elasticity, and the study of the impact of the loop type (a_0 <100> or ½ a_0 <111>), radius, its depth within the thin film and the anisotropy ratio on the elastic fields and energy of the thin film are made. The methodology developed for the purpose and the subsequent results are presented here. The effect of the free surfaces on irradiation induced dislocation loops formed during TEM in-situ irradiation experiments in comparison to bulk irradiation is discussed.

2. Thin foil treatment method and application

By virtue of the free character of the surfaces of the thin foil, the total traction stress components should be zero at their position. The general methodology consists in generating separately, on the one hand, the so-called bulk elastic field, σ_{ij}^{∞}, due to the defect and, on the other hand, the so-called image elastic field, σ_{ij}^{image}, which is made to cancel out the bulk stress at the free surfaces (Fig. 1). Their addition results in the so-called total elastic field, which is the desired solution:

$$\sigma_{ij}^{total} = \sigma_{ij}^{image} + \sigma_{ij}^{\infty} \tag{1}$$

This can be best achieved in Fourier space, for both isotropic [21] and anisotropic [20] materials. The calculation scheme presented in detail in Ref. [20] of the anisotropic image elastic field of a defect in presence of a free surface is summarized in Fig. 2. It allows deriving the elastic fields, namely the displacement and stress fields, induced by the defect at any position within the thin foil. It consists in the following steps:

① Write an arbitrary image displacement field at the free surface in 2D Fourier space.
② Generate the arbitrary image stress field in Fourier space using 3D anisotropic Hooke's law. This image stress field, σ_{ij}^{image}, is a 2D discrete Fourier series written with unknown 2D discrete Fourier coefficients.
③ Calculate the bulk stress σ_{ij}^{∞} of the defect at the free surfaces with any known elastic models.
④ Perform the 2D discrete Fourier transformation of the bulk stress, which results in corresponding 2D discrete Fourier coefficients.
⑤ Match the bulk stress field and image stress field in 2D discrete Fourier space, so as to satisfy the free traction stress condition $\sigma_{i3}^{\infty} + \sigma_{i3}^{image} = 0$ at the free surface.
⑥ Produce the 2D discrete Fourier coefficients for the arbitrary image displacement field in Fourier space.
⑦ Perform inverse 2D discrete Fourier transformation, thus producing the image elastic fields, namely the displacement, displacement gradient, and stress fields, in real space.

For a thin foil with arbitrarily oriented crystal surfaces, the following anisotropic image displacement field (u, v, w) in the 3D space (x, y, z) described in a 2D Fourier space is employed [20]:

$$\begin{cases} u = \sum_{k_x}\sum_{k_y}\left[U^S sinh\left(q^S \cdot z\right) + U^A cosh\left(q^A \cdot z\right)\right] \cdot exp\left(ik_x x + ik_y y\right) \\ v = \sum_{k_x}\sum_{k_y}\left[V^S sinh\left(q^S \cdot z\right) + V^A cosh\left(q^A \cdot z\right)\right] \cdot exp\left(ik_x x + ik_y y\right) \\ w = \sum_{k_x}\sum_{k_y}\left[W^S cosh\left(q^S \cdot z\right) + W^A sinh\left(q^A \cdot z\right)\right] \cdot exp\left(ik_x x + ik_y y\right) \end{cases} \tag{2}$$

where k_x and k_y are the Fourier coefficients and the third dimension is explicit with z. In addition, one has to consider the presence of the two free surfaces of the thin film. This is depicted in the following by an upper index '+' and '-' for respectively the upper and lower free surface. As the geometry is symmetrical by reflection against the x–y plane going through the middle of the thin foil, appropriate linear combinations of these traction and displacement vectors on the top and bottom surfaces can be performed. The equilibrium equations at the position along z of the free surfaces can be rewritten into two independent sets of equations on (U^S, V^S, W^S) and (U^A, V^A, W^A), the symmetric and the asymmetric part respectively. Then, three roots (q_1^S, q_2^S, q_3^S) and three roots (q_1^A, q_2^A, q_3^A) for the symmetric and asymmetric matrix equations can be calculated, respectively to these parts.

The symmetric image displacement solution u^S can be written as:

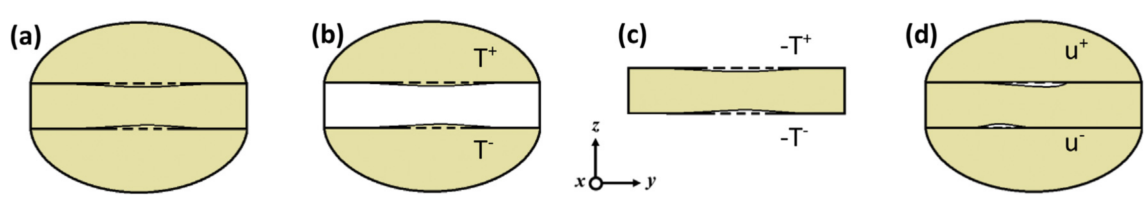

Fig. 1. Schematics illustrating the procedure to derive the elastic fields induced by a defect in a thin foil. (a) Infinite bulk material containing a defect in the center: the planned free surfaces (solid lines) of the thin foil that will be cut in the bulk are bent by the presence of the defect. (b) The two infinite half spaces outside of the thin foil present an elastic field that is equal in magnitude as the elastic field induced by the defect in the bulk material, but in opposite direction. (c) The thin foil containing the defect present an elastic field that is equal in magnitude as the elastic field induced by the defect in the bulk. (d) the defect-containing foil with free surfaces. After releasing the stress fields in (b) and (c), there are no applied external forces, but there will be a displacement across the surfaces of thin foil, as shown in (d).