Acta Materialia 99 (2015) 392–401

Contents lists available at ScienceDirect

Acta Materialia

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

Interactions of prismatic dislocation loops with free surfaces in thin foils of body-centered cubic iron

Jan Fikar *, Roman Gröger

Central European Institute of Technology & Institute of Physics of Materials (CEITEC IPM), Academy of Sciences of the Czech Republic, Žižkova 22, 616 62 Brno, Czech Republic

ARTICLE INFO

Article history:
Received 23 January 2015
Revised 30 July 2015
Accepted 31 July 2015

Keywords:
Dislocation loop
Dislocation mobility
Dislocation theory
Irradiation effect

ABSTRACT

We employ molecular statics simulations to investigate the interactions of circular and hexagonal $1/2\langle 111\rangle$ prismatic loops in body-centered cubic iron with two parallel $\{111\}$ free surfaces of a free-standing foil. If the presence of two surfaces is taken into account, these results agree well with the isotropic elastic solutions of Bastecka (1964) for circular loops and of Groves and Bacon (1970) for square loops with the Burgers vector of the loop perpendicular to the surface. By varying the size and shape of the loop, we identify the critical depth at which the image stresses overcome the internal lattice friction and thus drive the loop towards the surface. We investigate how this depth and the corresponding critical stress on the dislocation depend on the shape and size of the loop and outline how these results can be used to correct transmission electron microscope (TEM) measurements of the densities of prismatic dislocation loops in thin foils. For example, for the loops of 5 nm in diameter in a 50 nm thick foil, the loop density corrected for the existence of denuded zones adjacent to the surfaces of the foil is shown to be nearly 49% higher than that obtained by direct TEM measurements.
© 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

1. Introduction

Prismatic dislocation loops [1,2] in body-centered cubic (BCC) metals are under intensive study, which is mainly driven by the recent European Fusion Development Agreement (EFDA) effort to find suitable materials for future fusion reactors. TEM observations of ion irradiated BCC Fe reveal a population of dislocation loops with Burgers vectors $1/2\langle 111\rangle$ and $\langle 100\rangle$ [3,4]. Upon irradiating a thin single-crystalline foil of Fe, $\langle 100\rangle$ loops dominate at temperatures higher than about 400 °C [5–7]. Theoretically $1/2\langle 111\rangle$ loops are most stable in Fe at temperatures under 350 °C, while at higher temperatures $\langle 100\rangle$ loops become predominant [8]. However, TEM observations of Fe samples irradiated at room temperature showed mixed $1/2\langle 111\rangle$ and $\langle 100\rangle$ loop populations, where the latter dominated the microstructure [4,9]. Although $\langle 100\rangle$ loops were observed in Fe long time ago [3], there is still no agreement on the mechanism of their formation at low temperatures. In principle, they are formed from individual interstitials or interstitial clusters, but the underlying process is not well understood. There are several theories how $\langle 100\rangle$ loops can be created from $1/2\langle 111\rangle$ loops [10–12], but none of them is widely accepted. Because the mechanism of the loop escape via the free surface of a TEM foil is not known, interpretations of experimental observations are not guaranteed to be quantitatively accurate.

It is worthwhile noting that $\langle 100\rangle$ loops are significantly less mobile than the $1/2\langle 111\rangle$ loops [13]. Molecular dynamics (MD) simulations show that larger interstitial clusters form $1/2\langle 111\rangle$ perfect prismatic dislocation loops that are highly mobile (migration barrier below 0.1 eV) and undergo a rapid one-dimensional movement on their glide cylinder [14,15]. The high mobility of $1/2\langle 111\rangle$ loops is the key property that allows for the evolution of the microstructure under irradiation. Nevertheless, the high mobility of prismatic loops introduces uncertainties into the estimates of loop densities in irradiated TEM samples, which typically arise due to neglecting the surface-enhanced mobility of the loops in thin foils. Since the thicknesses of TEM foils transparent to the electron beam are typically less than a hundred nanometers, the prismatic loops are attracted by free surfaces and can easily escape from the foil owing to low Peierls stresses of edge dislocations in BCC metals. Only the loops beyond a certain minimum depth from the surface can thus remain in the sample and be detected by TEM. For example, in the case of irradiation-induced dislocation loops with diameters 2–10 nm in Fe at 300 °C, this threshold depth was estimated to be as large as 20–25 nm [5]. Prokhodtseva et al. [9,16] made an attempt to quantify the effect of the free surface by comparing the microstructure of thin TEM foils irradiated in situ with that of irradiated bulk samples, where the TEM

* Corresponding author.
E-mail address: fikar@ipm.cz (J. Fikar).

http://dx.doi.org/10.1016/j.actamat.2015.07.077
1359-6454/© 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

lamellae were extracted post-mortem by focused ion beam (FIB). The quantity and morphology of observed dislocation loops were found to depend on whether free surfaces were present or absent. These observations provide ample evidence that the results obtained on thin TEM foils may not be representative of the bulk material.

The theoretical derivation of the equilibrium elastic solution of a circular prismatic loop with its Burgers vector perpendicular to the free surface of an isotropic semi-infinite medium was made by Bastecka [1]. While this derivation is directly applicable to nearly elastically isotropic materials, it is not clear to what extent it applies to anisotropic materials of which Fe is one of the most important representatives. A similar derivation was made for square prismatic loops by Groves and Bacon [2], where only the forces at the midpoints of the four linear segments of the loop with the Burgers vector perpendicular to the free surface were considered. The theoretical formula of Groves for square loops was found to be applicable also to circular loops in MgO with the Burgers vector $1/2\langle 1\,1\,0\rangle$ [17]. No attempt was made so far to investigate how free surfaces affect the mobility of the prismatic loop and how this changes for non-circular loops and for the loops not parallel to the surface. The only exceptions are several computationally expensive dynamical spectral Fourier transform methods for calculating image forces on dislocation segments close or even intersecting the free surface. While these can be used with discrete dislocation dynamics calculations [18–20], they are not easily applicable to TEM studies of dislocation loops.

The objective of this paper is to investigate the stresses that arise due to the interactions of $1/2\langle 1\,1\,1\rangle$ prismatic loops with free surfaces. For a range of sizes of circular and hexagonal prismatic loops, we determine the critical stress exerted on the loop by its images at which the loop escapes to the free surface. The critical position of the loop at this instability is used to estimate the thickness of denuded (i.e. loop-free) zones below the two free surfaces. We demonstrate that the knowledge of the size of these denuded zones is essential for quantitatively correct predictions of the densities of prismatic dislocation loops. These results can be directly used to estimate the kinetics of recovery of irradiated free-standing foils.

2. Theoretical background

Bastecka [1] was the first to derive the force on a circular prismatic loop positioned in a finite depth below the surface of a semi-infinite elastic body. The plane of the loop was parallel to the surface and thus the Burgers vector of the loop was perpendicular to the surface. Solving the equilibrium problem in the framework of the elasticity theory, Bastecka obtained the force $\mathbf{f}$ that the surface exerts on a unit length of the loop. This force is perpendicular to the surface (parallel to her x_3 axis) and thus $\mathbf{f} = f_{3B}\hat{\mathbf{e}}_3$, where $\hat{\mathbf{e}}_3$ is a unit vector parallel to x_3. Accounting for a missing multiplication by $2/\pi$ in Eq. (11) of Bastecka [1], the force per unit length of the loop can be written as:

$$f_{3B}(a) = \frac{1}{8\pi}\frac{b^2\mu}{R(1-\nu)}\frac{1}{\left(\sqrt{1+d^2}\right)^5} \times \left[\frac{-3d^4+7d^2+2}{d}E\left(\frac{1}{1+d^2}\right) + d(3d^2-1)K\left(\frac{1}{1+d^2}\right)\right]. \quad (1)$$

Here, a is the distance (depth) of the loop from the surface, R the loop radius, $d = a/R$, b the magnitude of the Burgers vector of the loop, μ the shear modulus, ν the Poisson ratio, and E, K the complete elliptic integrals of the first and second kind, respectively. It is important to emphasize that Bastecka uses the elliptic integrals $E_0(k)$ and $K_0(k)$, while (1) uses equivalent representations $E(M)$ and $K(M)$, where $M = k^2$ (see [21]).

A similar expression was obtained later by Groves and Bacon [2] for a square prismatic loop in a half-space terminated by the free surface perpendicular to the Burgers vector of the loop. Here, only the forces at the midpoints of the linear loop segments are considered. The force on the square loop is then given by the formula:

$$f_{3G}(a) = \frac{1}{4\pi}\frac{b^2\mu m}{c(1-\nu)} \times \left[\frac{m^2+40m+768}{(m+16)^{5/2}} + \frac{16(105m^3+460m^2-544m-3072)}{(m+4)^3(5m+16)^{5/2}}\right]. \quad (2)$$

Here, c is the edge length of the square loop and $m = c^2/a^2$; these are denoted in [2] as h and y, respectively. From the condition of equivalence of surfaces of the circular and square loops [22], i.e. $\pi R^2 = c^2$, and employing the definition of m above, we arrive at an expression $m_{equiv} = \pi/d^2$. The corresponding edge length of this equivalent square loop is $c_{equiv} = (a/d)\sqrt{\pi}$. It is interesting to note that (2) with m replaced by m_{equiv} gives forces on the square loop that are surprisingly similar to those for circular loops of radius R obtained from (1); this is shown in Table A1.

These derivations can be extended to obtain the force on a prismatic dislocation loop located in a foil of thickness h. Since the force fields represented by (1) and (2) decay rapidly with increasing depth of the loop a, the solution for large h can be obtained as a direct superposition of the forces obtained from the solutions in half-space. In particular, we consider a configuration, where the distance from the loop to the upper surface is a_1 and to the lower surface a_2 so that the foil thickness is $h = a_1 + a_2$. The force on the loop at the position y measured from the middle-plane of the foil (Fig. 1) due to its image at the position $y' = 2a_1$ measured from the position of the loop is $f_3(a_1)$ and the force exerted on the loop by the image at $y' = -2a_2$ is $f_3(-a_2) = -f_3(a_2)$ because f_3 is odd with respect to a and d and both images have Burgers vectors $-\mathbf{b}$. Here, f_3 represents any of the two forces in (1) and (2). Hence, the combined force of the two images acting on the loop at the position y is $f_3^{(0)}(y) = f_3(a_1) - f_3(a_2)$. The total force exerted by image forces on the loop is an infinite series of which $f_3^{(0)}$ is the leading term. The first-order correction can be obtained by considering the image with the Burgers vector $+\mathbf{b}$ at $y'' = -2h$ that is obtained from the previous image at $y' = 2a_1$; this exerts the force on the loop $-f_3(h)$. The other image is at $y'' = 2h$ and the corresponding force on the loop is $f_3(h)$. The combined action of these two forces on the loop is then $f_3^{(1)}(y) = f_3(h) - f_3(h) = 0$ and thus the first-order correction does not contribute to the sum. In a similar manner, all odd order terms vanish. The second-order term due to the image dislocation with the Burgers vector $-\mathbf{b}$ is $f_3^{(2)}(y) = f_3(h+a_1) - f_3(h+a_2)$. The force on the dislocation loop can thus be represented by an infinite series:

$$f_3^{\Sigma}(y) = \sum_{k=0}^{\infty} f_3^{(2k)}(y) = \sum_{k=0}^{\infty}[f_3(kh+a_1) - f_3(kh+a_2)]. \quad (3)$$

If $a_1 < a_2$, i.e. the loop is in the upper half of the foil ($y > 0$ in Fig. 1), the term with $k = 1$, i.e. $f_3(h+a_1) - f_3(h+a_2)$, is smaller than $f_3(h+a_1)$. For the range of foil thicknesses and the largest loop considered in this paper, the latter represents only about 5 meV in the interaction energy and 30 Pa in the critical stress. The force on the loop can thus be safely approximated as $f_3^{\Sigma} \approx f_3(a_1) - f_3(a_2)$. However, more terms in (3) may need to be used for very thin foils and/or very large loops, where R is not much smaller than h. In this

Download English Version:

https://daneshyari.com/en/article/7879625

Download Persian Version:

https://daneshyari.com/article/7879625

Daneshyari.com