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Interaction of irradiation-induced prismatic dislocation loops with free surfaces in tungsten

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ABSTRACT

The prismatic dislocation loops appear in metals as a result of high-energy irradiation. Understanding their formation and interaction is important for quantification of irradiation-induced deterioration of mechanical properties. Characterization of dislocation loops in thin foils is commonly made using transmission electron microscopy (TEM), but the results are inevitably influenced by the proximity of free surfaces. The prismatic loops are attracted to free surfaces by image forces. Depending on the type, size and depth of the loop in the foil, they can escape to the free surface, thus invalidating TEM observations and conclusions. In this article small prismatic hexagonal and circular dislocation loops in tungsten with the Burgers vectors $1/2\langle 1\,1\,1\rangle$ and $\langle 1\,0\,0\rangle$ are studied by molecular statics simulations using three embedded atom method (EAM) potentials. The calculated image forces are compared to known elastic solutions. A particular attention is paid to the critical stress to move edge dislocations. The escape of the loop to the free surface is quantified by a combination of atomistic simulations and elastic calculations. For example, for the $1/2\langle 1\,1\,1\rangle$ loop with diameter 7.4 nm in a 55 nm thick foil we calculated that about one half of the loops will escape to the free surface. This implies that TEM observations detect only approx. 50% of the loops that were originally present in the foil.

1. Introduction

Transmission electron microscope (TEM) studies of low-dose irradiated tungsten foils revealed the presence of prismatic dislocation loops with Burgers vectors $1/2\langle 1\,1\,1\rangle$ and $\langle 1\,0\,0\rangle$ of which the $1/2\langle 1\,1\,1\rangle$ loops are dominating [1]. Irradiation at room temperature shows a lot of small loops (2.07 nm average diameter) and no large loops. On the other hand, irradiation at 800 °C produces only large loops (7.55 nm average diameter). From these results, we have estimated that the number of point defects needed to create the loops visible in TEM is surprisingly the same at both temperatures.

Recent high-energy and low-energy tungsten irradiation experiments show variations of the relative number of $1/2\langle 1\,1\,1\rangle$ and $\langle 1\,0\,0\rangle$ loops. High-energy irradiation uses 2 MeV self-ions with damage peak depth 75 nm, which is thus a near-bulk irradiation [2]. On the other hand, low-energy irradiation uses 150 keV self-ions with damage peak depth only 15 nm [3]. In the case of near-bulk irradiation almost double the ratio of the numbers of $1/2\langle 1\,1\,1\rangle$ to $\langle 1\,0\,0\rangle$ loops is found when compared to the low-energy irradiation, because in the latter case many mobile $1/2\langle 1\,1\,1\rangle$ loops are created close to the free surface and can thus escape.

The elastic solution of the equilibrium problem of a circular loop with the Burgers vector perpendicular to the free surface was found by Baštecká [4].[1] A similar procedure was later used by Groves and Bacon [6] to derive the elastic solution for a square prismatic loop. Despite different shapes of the loops, the forces acting on them, predicted by both models, are surprisingly close to each other. We have recently developed a general method for calculating the critical depth of a prismatic loop from the critical stress and elastic constants and applied it to body-centered cubic (BCC) iron [5]. Based on these calculations, we have proposed a simple method to account for the existence of denuded zones adjacent to the surfaces of the foil, which allows for quantitative TEM studies of the densities of prismatic dislocation loops.

The objective of this paper is to follow up on these calculations by carrying our a series of atomistic studies on $1/2\langle 1\,1\,1\rangle$ and $\langle 1\,0\,0\rangle$ dislocation loops. In all calculations, the plane of the loop is always

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[1] This paper contains a few misprints that we have corrected in Ref. [5].

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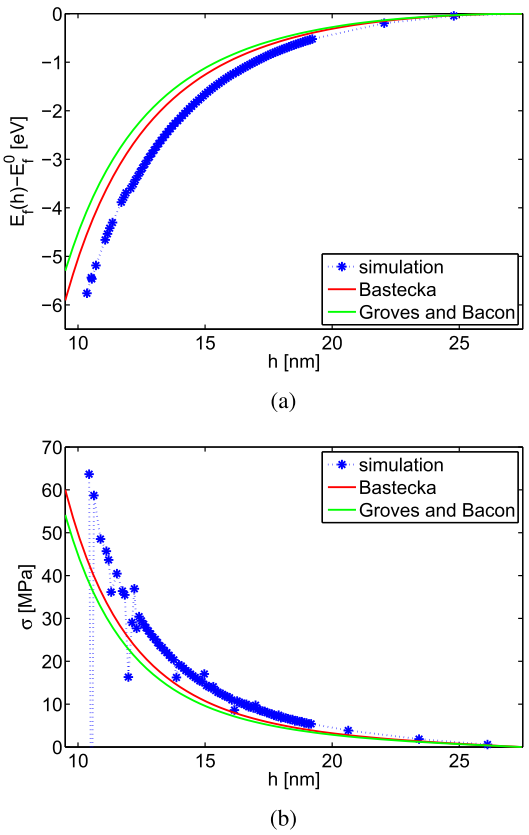

Fig. 1. (a) Dependence of the formation energy of a circular $1/2\langle 111\rangle$ loop created by 397 atoms and relaxed using the *AT* potential on the loop depth. (b) Variation of the image stress acting on the loop with the loop depth.

parallel to the foil surface and the Burgers vector perpendicular to it. Using three embedded atom method (EAM) potentials for tungsten, we determine how the formation energy and stresses exerted on the loop by their images depend on the position of the loop below the surface. Comparing these dependencies with the predictions of simplified elastic solutions [4,6] provides an important insight into the effect of inelastic relaxations on the stability of prismatic dislocation loops in irradiated tungsten foils.

2. Computational details

Let us consider a bulk-like cuboidal simulation block with periodic boundary conditions in all directions. The equilibrium configuration of the dislocation loop is obtained by inserting the loop into the middle of the block by the procedure described in Ref. [5] and relaxing all atoms. A number of slabs of a fixed thickness but different distance of the loop to the two surfaces are then cut from the block to produce free-standing foils with the loop in different depths below the surfaces. Caution is needed when the loop is close to any of the two surfaces, which leads to bulging of atomic planes close to the loop. This may cause the number of atoms in the foil to vary. Nevertheless, such short distances are usually not of interest, because they are very small compared to the critical depth from which the loop escapes at 0 K.

The thickness of the foil is set to $200b$ for $\boldsymbol{b} = 1/2\langle 111\rangle$ and $173b$ for $\boldsymbol{b} = \langle 100\rangle$, i.e. approximately 54.7 nm, which is the typical thickness of TEM foils. We investigated three sizes of the loops: small, medium, and large with diameters 1.78 nm, 5.54 nm, and 7.42 nm, respectively (they are created by inserting approximately 37, 397, and 721 atoms as described in Ref. [5]). The small and large loop diameters agree well with experimental observations [1]. The loops are created such that their area is parallel and their Burgers vectors perpendicular to the two surfaces of the foil. The simulated loops have either hexagonal or circular shape. In tungsten, the $1/2\langle 111\rangle$ loop has the lowest formation energy if possessing the hexagonal shape, whereas the $\langle 100\rangle$ loop prefers to be circular [7]. For very mobile $1/2\langle 111\rangle$ loops, we consider both hexagonal and circular shapes. The former contains only $\{110\}$ segments, while the latter has not only $\{110\}$ but also $\{112\}$ segments that are harder to move. In the case of $\langle 100\rangle$ loops, we expect very large stresses to move the loop and, simultaneously, a weaker dependence of mobility on the loop shape.

In our atomistic simulations, we use three different EAM potentials: (i) the potential of Ackland and Thetford (*AT*) [8]; this yields practically the same results as the Finnis–Sinclair potential in [9], (ii) the *EAM-4* potential developed in the paper by Marinica et al. [10][2] that we designate here as *M4*, and (iii) the potential of Wang et al. (*W*) [11]. The often used potential of Derlet et al. (*D*) [12] has

Table 1
The geometry and size of the loops used for the simulations using the *AT* potential. The loop diameter is d, the calculated critical depth h_c, and the critical image stress σ_c.

$\boldsymbol{b}$	$1/2\langle 111\rangle$			$\langle 100\rangle$	
Size	Small	Medium	Big	Medium	Medium
Atoms	37	397	721	397	401
d [nm]	1.78	5.54	7.42	5.54	5.22
Shape	Hexa	Hexa	Hexa	Circ	Circ
h_c [nm]	4.7	11.2	13.9	10.4	2.4
σ_c [MPa]	50	38	43	58	2300

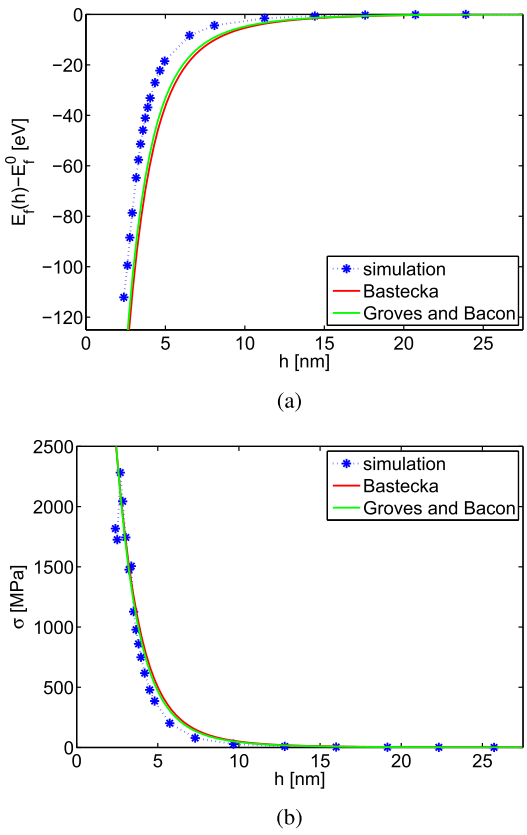

Fig. 2. Variation of (a) the formation energy of the loop, and (b) the image stress acting on the loop with the loop depth. The results were obtained using the *AT* potential for a circular $\langle 100\rangle$ loop created by 401 atoms.

[2] This is denoted as *MVG3* in [9].