Distinguishing screw dislocation core configuration in bcc W using TEM

R. Schäublin[1], J. Fikar[1]

1. Ecole Polytechnique Fédérale de Lausanne (EPFL), Centre de Recherches en Physique des Plasmas, Association Euratom-Confédération Suisse, 5232 Villigen PSI, Switzerland

robin.schaeublin@psi.ch
Keywords: bcc metal, screw dislocation, molecular dynamics simulation, TEM

Plasticity of bcc metals is governed at low and intermediate temperatures by the mobility of the ½ a_0 <111> screw dislocation. Indeed, its non planar core structure, as opposed to the planar core configuration of the edge dislocation, makes it difficult to move in the lattice without costly constriction onto one of the {110} glide planes. It has been postulated long ago [1] and confirmed later by molecular dynamics simulations [2] that the core should have a 3-fold symmetry, developing onto three conjugate {110} planes around the <111> dislocation line. In detail, this development might lead to either a symmetrical configuration, giving rise to a 6-fold symmetry, or a degenerate configuration, which is asymmetrical [3]. In addition, depending on the exact location of the dislocation in the lattice, it is either relatively easy or hard to move it with an external shear stress, thus resulting in the naming of easy or hard core, respectively. This is critical to understand hardening due to irradiation-induced damage, as dislocations progress only when their screw parts due to bowing at pinning defects can start to move [4]. However, there are until now only few experimental TEM observations supporting these theoretical descriptions, as e.g. the one of Sigle in Mo [5], suggesting the 3-fold symmetry, with a view of the dislocation end on by HR-TEM. Others have searched by image simulation conditions of end on TEM observation of the screw dislocation in Mo [6]. They notice that the Eshelby twist of the thin foil due to the free surfaces renders the end on observation of the screw dislocation difficult [6].

We explore the possibility to distinguish by TEM the various screw dislocation cores in W, taken as model bcc metal for its large lattice parameter (3.165 Å), using molecular dynamics simulation [8]. Figure 1 shows 4 possible cores. For that purpose we try TEM diffraction contrast of the dislocation laying nearly parallel in the foil instead of end on, in order to minimize the free surface effects. Images are simulated using the many beam technique with the CUFOUR code [7]. The description of the screw dislocation based on isotropic elasticity is made using a novel analytical description allowing for the degeneracy of the core. It is controlled by a free parameter [8]. Simulations show that in bright field there are differences, though minute, allowing for the distinction of the symmetrical core from the asymmetrical core (Figure 2). The approach appears to be extremely promising.

1. P.B. Hirsch, Proc. of the 5th. Int. Conf. of Crystallography, Cambridge University Press (1960) p. 139.
2. V. Vitek, Proc. R. Soc. Lond. A 352 (1976) p. 109
3. V. Vitek, Philosophical Magazine 84 (2004) p. 415
4. R. Schäublin, N. Baluc, Nuclear Fusion 47 (2007) p. 1690
5. W. Sigle, Phil. Mag. A, 79 (5) (1999) p. 1009
6. B.G. Mendis, K.J. Hemker, Ultramicroscopy, 108 (9) (2008) p. 855
7. R. Schäublin, P. Stadelmann, Materials Science and Engineering A, 164 (1993) p. 373
8. J. Fikar, R. Schäublin, Advanced Materials Research, 59 (2009) p. 247

W. Grogger, F. Hofer, P. Pölt (Eds.): MC2009, Vol. 3: Materials Science,
DOI: 10.3217/978-3-85125-062-6-472 , © Verlag der TU Graz 2009

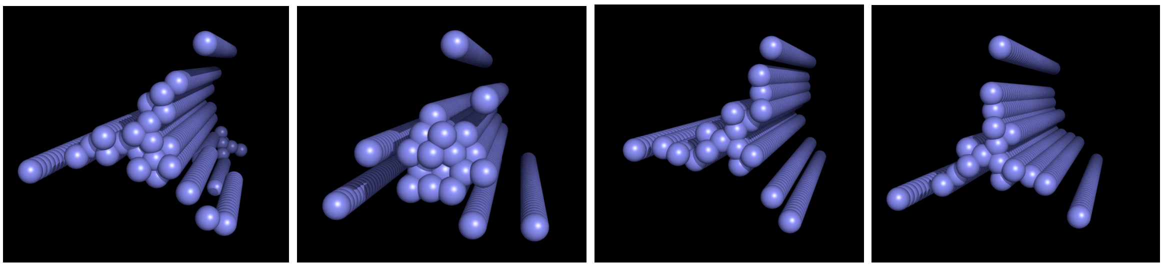

Figure 1. Atomistic description of possible screw dislocation cores in W viewed end on: (a) easy symmetrical, (b) easy degenerate, (c) hard symmetrical and (d) hard degenerate configuration. Only atoms having a potential energy higher than -8 eV are shown.

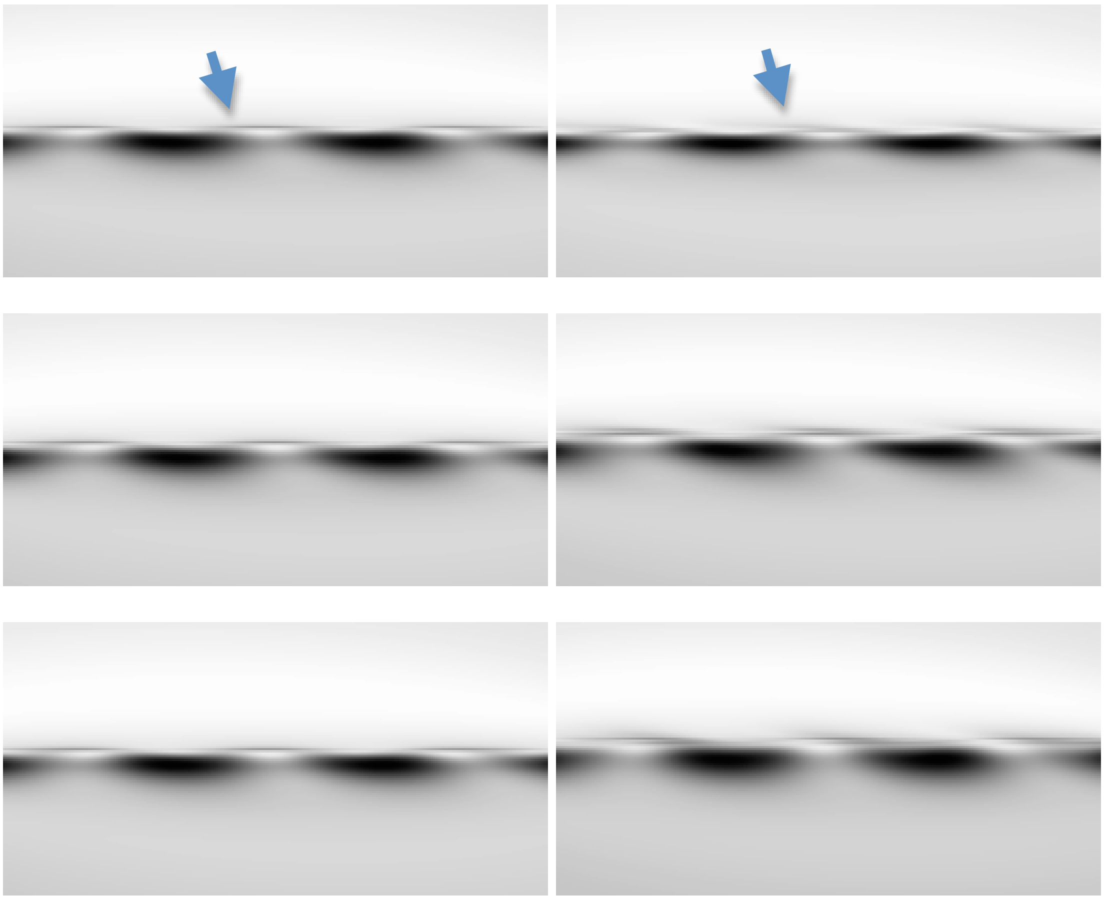

Figure 2. Simulated TEM bright field images of the screw dislocation in W, viewed perpendicular to the beam in the thin foil, according to a (left) symmetrical and (right) asymmetrical core configuration. Arrows point to regions of contrast differences between the symmetrical and asymmetrical core. Note the splitting of the central thin contrast line only for the asymmetrical core. From top to bottom the dislocation core is rotated relative to the beam direction $[1\bar{1}0]$. Top row: 0°, middle row: 30° and bottom row: 60°. Imaging conditions: 200 kV, foil normal: $[2\bar{1}0]$, dislocation direction: [111], diffraction vector g: (222), diffraction condition: 0g(1.05g). Individual image width: 65 nm.

W. Grogger, F. Hofer, P. Pölt (Eds.): MC2009, Vol. 3: Materials Science,
DOI: 10.3217/978-3-85125-062-6-472 , © Verlag der TU Graz 2009