Journal of Nuclear Materials 386–388 (2009) 115–118

Contents lists available at ScienceDirect

Journal of Nuclear Materials

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

# Molecular dynamics simulation of dislocation–void interactions in BCC Mo

Hyon-Jee Lee *, Brian D. Wirth

*Department of Nuclear Engineering, University of California, Berkeley, CA, USA*

A B S T R A C T

Molecular dynamics (MD) and molecular statics (MS) simulations have been performed to simulate the motion of a screw dislocation and its interaction with voids in irradiated body centered cubic (BCC) Mo. Considering the unique non-planar core structures of the screw dislocation in BCC metals, the behavior of screw dislocation motion as a function of temperature and applied shear stress is first discussed. A transition from smooth to rough motion of the screw dislocation is observed with increasing shear stress, as well as a change of dislocation glide plane from {1 1 0} to {1 1 2} with increasing temperature. The interaction of a screw dislocation with nanometer-sized voids observed in both dynamic and static conditions is then reported. The obstacle strength calculated from MS calculations shows a large increase in critical resolved shear stress for void diameter larger than about 3 nm. However, the MD results indicate that the screw dislocation interaction with void occurs via a simple shear mechanism.



## 1. Introduction

The irradiation of structural materials in nuclear environments can produce radiation induced defects and significant mechanical property changes, including yield stress increases and ductility decreases. Depending on material and irradiation conditions, the defect population varies from small point defect clusters to dislocation loops, voids, helium bubbles, and radiation-induced precipitates. Transmission electron microscopy (TEM) deformation studies of irradiated materials showed that these defects act as obstacles to dislocation motion, thus changing the local deformation behavior. However, detailed knowledge of the interaction mechanisms between a dislocation and radiation induced obstacles is difficult to obtain by post situ and even in situ TEM methods.

In BCC metals, TEM studies indicate that screw dislocations control the plasticity at low temperature. While atomistic simulation methods can provide the sequence-of-events controlling the interaction between a dislocation and an obstacle, the screw dislocation interaction with radiation obstacles in BCC metals has not been extensively studied using MD methods, presumably because of the more complex motion of screw dislocations in BCC metals by kink pair formation, which shows a smooth to rough transition [1]. Typical defects in BCC Mo are mostly dislocation loops and small voids at lower irradiation temperature, whereas only voids are observed at higher temperatures [2]. Previous analytical work on void strength indicates that the void is a very strong obstacle and the bypassing stress can approach the Orowan stress for impenetrable obstacles [3]. Thus a clear understanding and reliable estimate of their strengthening effect is important for evaluating performance of BCC Mo under irradiation conditions.

In this paper, we present atomistic simulations results that investigate the interaction between screw dislocations and voids in BCC Mo. Considering the unique non-planar core structure of the screw dislocation, we first present the behavior of screw dislocation motion in BCC Mo. Conjugate gradient MS simulation results are presented that quantify the energetics of void shearing. As well, dynamic detachment behavior is studied using MD simulations.

## 2. Simulation methods

The MD simulations have been performed using a modified version of the MDCASK code [4], implemented with the Finnis–Sinclair N-body potential to describe the atomic interactions in BCC Mo [5]. It should be noted that the screw dislocation core in BCC Mo in Finnis–Sinclair potential is degenerate, but numerous recent studies based on tight-biding or density functional theory (DFT) calculations predicts a non-degenerated core [6–9], suggesting that different behaviors might be expected depending on the dislocation core type. However, both degenerate and non-degenerate core structures become a degenerate core upon applied shear stresses, hence the trend of results presented here should remain valid for both core structures [10]. The simulation cell consists of a body centered cubic lattice, bounded by $(1\,\bar{1}\,0)$, $(1\,1\,1)$, and $(\bar{1}\,\bar{1}\,2)$ faces in $X = a_0[1\,\bar{1}\,0]$, $Y = a_0/2[1\,1\,1]$, and $Z = a_0[\bar{1}\,\bar{1}\,2]$ directions, respectively. The size of the BCC Mo simulation cell is $60 \times 100 \times 60$ unit cells, approximately $27 \times 27 \times 46$ nm ($X$, $Y$ and $Z$ directions), and contains about 2.2 million atoms. Periodic boundary conditions are applied in the $Y$ and $Z$ directions. The $X$ surface is initially free, but is subject to a shear stress ranging from 0.7 to 4 GPa following

* Corresponding author.
*E-mail address:* hyon-jee@nuc.Berkeley.EDU (H.-J. Lee).

0022-3115/$ - see front matter © 2009 Elsevier B.V. All rights reserved.
doi:10.1016/j.jnucmat.2008.12.084

equilibration. The simulation temperature is set to a corresponding temperature at an equilibration stage and not controlled further. A screw dislocation with $\boldsymbol{b} = a_0/2[1\,1\,1]$ is introduced using the elastic isotropic displacement field. The void is introduced into the simulation cell by removing atoms of spherical region.

The conjugate gradient MS simulations with a screw dislocation and a void of diameter from 1.5 to 5 nm have been performed to calculate the critical resolved shear stress and obstacle strengths as a function of a void size. The simulation cell size ranging in size from $20 \times 50 \times 20$ to $20 \times 150 \times 20$ and $60 \times 100 \times 60$ unit cells have been used to determine the effects of cell size and void spacing.

## 3. Results and discussion

### 3.1. Screw dislocation motion

The screw dislocation core structure in BCC Mo is degenerate (N and P type [11]), with core spreading into three $\{1\,1\,0\}$ planes along $\langle 1\,1\,2\rangle$ directions as anticipated with a Finnis–Sinclair potential [10]. At $T = 100$ K and an applied shear stress of 1 GPa, screw dislocation motion occurs through the double kink nucleation and propagation mechanism, which agrees with the previous simulation results in BCC Fe at low temperature and low stress [1,12]. The motion is relatively smooth but does involve cross-slip, thus the dislocation trajectories appear wavy and non-crystallographic. Close examination of dislocation displacement (DD) map suggests that such cross-slip is favored after the dislocation core flip between N and P type. At a higher applied stress of 1.5 GPa, the dislocation again moves by a double kink nucleation and propagation mechanism, although the higher applied stress results in a larger rate of double kink nucleation. This leads to interactions amongst kinks, which are formed on different glide planes, that necessitate the formation of Frenkel pairs to resolve the topological constraint, as previously observed in BCC Fe [1,12]. The vacancies are immediately emitted from the dislocation as individual point defects, whereas the self-interstitial atoms are dragged along the dislocation core and form clusters of $\langle 1\,1\,1\rangle$-oriented self-interstitials (crowdions). The self-interstitial clusters are later emitted from the moving screw dislocation with a distribution of cluster sizes in the form of $\langle 1\,1\,1\rangle$ crowdion interstitial clusters and dislocation loops. Thus, the motion of the screw dislocation at high applied shear stresses results in the formation of a self-debris field marking the path of dislocation motion. When the applied shear stress is further increased to 4 GPa, the dislocation loops generated by the rough motion rapidly expand on $\{1\,1\,0\}$ planes and coalesce with other dislocation loops or itself through a periodic boundary as shown in Fig. 1. As a result, dislocation multiplication occurs in the simulation cell.

As well, a strong temperature dependence of screw dislocation motion is observed. As summarized in Fig. 2, the MD simulation results show that the screw dislocation glides in the $\langle 1\,1\,2\rangle$ direction on $\{1\,1\,0\}$ planes at $T < 250$ K, but switches to glide in the $\langle 1\,1\,0\rangle$ direction on $\{1\,1\,2\}$ planes at $T > 250$ K. At above $T = 250$ K, the screw dislocation moves on $\{1\,1\,2\}$ planes in the twinning direction. When the applied stress is low, smooth motion is observed. When the applied stress is increased, rough motion is observed. When the applied stress is further increased, the dislocation generates twin layers on $\{1\,1\,2\}$ planes. The twin layer formation is also observed in BCC Fe [1,12]. However, Marian et al. report no temperature dependency of the screw dislocation glide plane in BCC Fe [1], while Chassidon et al. reports only BCC Fe with non-degenerate core glides on $\{1\,1\,0\}$ plane at low temperature [12]. It should be noted that the core type of BCC Mo in this study is degenerate and thus different from the previous simulation results in BCC Fe.

### 3.2. Molecular statics (MS) study of screw dislocation interaction with void

The conjugate gradient MS simulations have been performed to obtain the equilibrium configurations, energetics and forces associated with the dislocation–void interactions at $T = 0$ K. These quantities provide the critical resolved shear stress and obstacle strengths required in constitutive models and provide a means of validating the interaction results obtained from high strain rate MD simulations.

The excess potential energy as a function of dislocation position relative to the void has been obtained from the conjugate gradient MS calculations as shown in Fig. 3(a). For void diameters between 1.5 and 5.0 nm, and void spacing of 50, 100 and 150 $b$, the critical resolved shear stress ($\tau_{CRSS}$) of a regular array of voids of different sizes is calculated using the following equation:

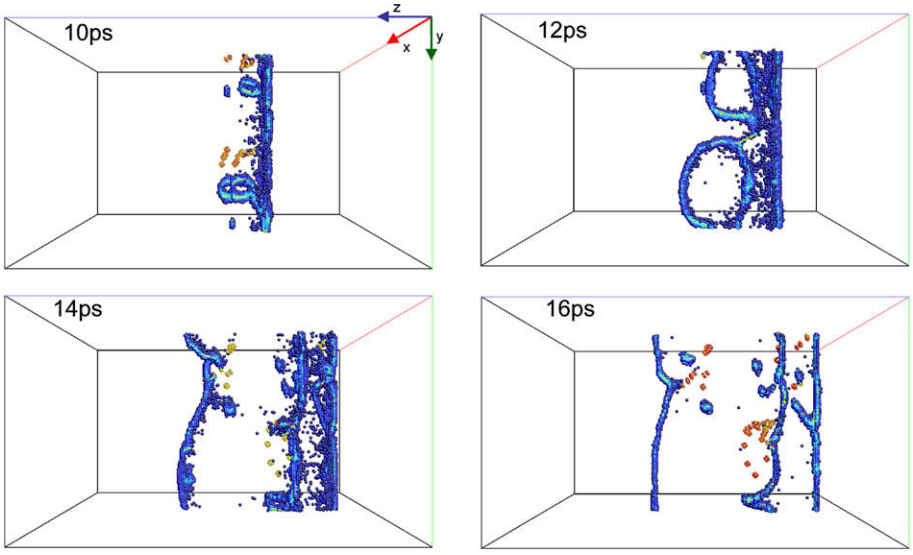


**Fig. 1.** Dislocation multiplication via loop generation. The MD snapshots of a dynamic sequence in which self-pinning leads to a dislocation loop generation, growth, coalescence, and dislocation multiplication. The simulation temperature is 100 K and the applied shear stress is 4 GPa.

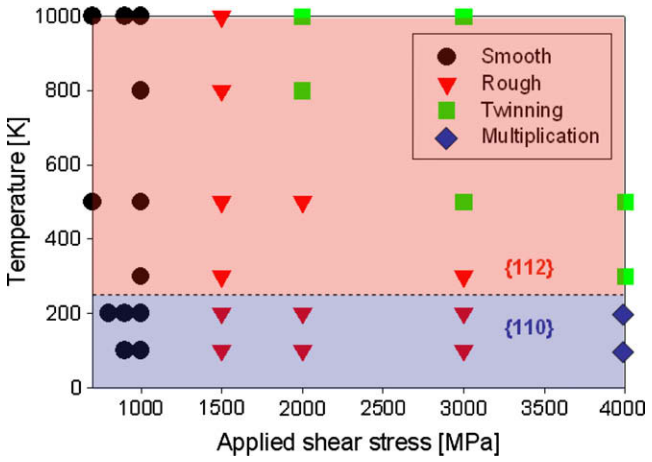


**Fig. 2.** Deformation map of BCC Mo as a function of temperature and applied shear stress. At $T < 250$ K, the dislocation glides on {1 1 0} plane while it glides on {1 1 2} plane at $T > 250$ K. A smooth to rough transition occurs with increasing the applied shear stress increases. Upon further increase of the stress, dislocation multiplication is observed at $T < 250$ K, while the twinning on {1 1 2} planes is observed at $T > 250$ K.

$$\tau_{CRSS} = \frac{F_{max}}{b(L-D)} \approx \frac{\Delta E_{max}}{\Delta x} \cdot \frac{1}{b(L-D)}, \quad (1)$$

where $F_{max}$ is the maximum force exerted by the void against dislocation shear, as numerically evaluated from the potential energy vs. distance calculations, $b$ is the dislocation Burgers vector amount, $L$ is the inter-particle (void) spacing along the dislocation line and $D$ is the void diameter [13]. Notably, a significant increase in the predicted critical resolved shear stress occurs for void sizes larger than about 3 nm in diameter as shown in Fig. 3(b). Interestingly, MD simulations in Cu by Hatano and Matsui show similar behavior for dislocation–nanovoid pinning, showing an abrupt increase of the critical stress of the leading partial when the void diameter is larger than 2 nm [14].

To understand the large increase in critical resolved shear stress for void diameters above about 3 nm, the values obtained from Eq. (1) have been compared to the Orowan stresses for the void and screw dislocation interaction, and are shown in Fig. 4. The cross-over between shear and Orowan mechanism occurs at around the void diameter ($D$) about 3 nm. Thus, it is tempting to conclude that this indicates a change in detachment mechanism from shear to an Orowan like mechanism. Osetsky et al have previously reported an Orowan like behavior in an edge dislocation detaching from a void in BCC Fe at $D \geqslant 1$ nm [15]. Therefore, to observe the dynamic interaction behavior between a screw dislocation and a void, MD simulations were performed (following section).

### 3.3. MD study of screw dislocation interaction with void

To determine the dynamic critical resolved shear stress as a function of the void size and the detachment mechanism of a screw dislocation from a void, MD simulations are performed. At low temperature ($T = 100$ K), the dislocation glides on {1 1 0} plane with frequent cross-slip. Thus, in general, the {1 1 0} plane that dislocation enters the void is not identical to the plane that detachment occurs. The dislocation bends towards to the void when it nears the void due to the attractive interaction, and it start to annihilate upon contact with the void. During the detachment, the annihilated dislocation segments re-nucleate on the exit surface of the void, while the other dislocation segments continue to glide. The detachment angle appears to be larger than 90 degrees in all cases, suggesting that the void is not a very strong obstacle against a

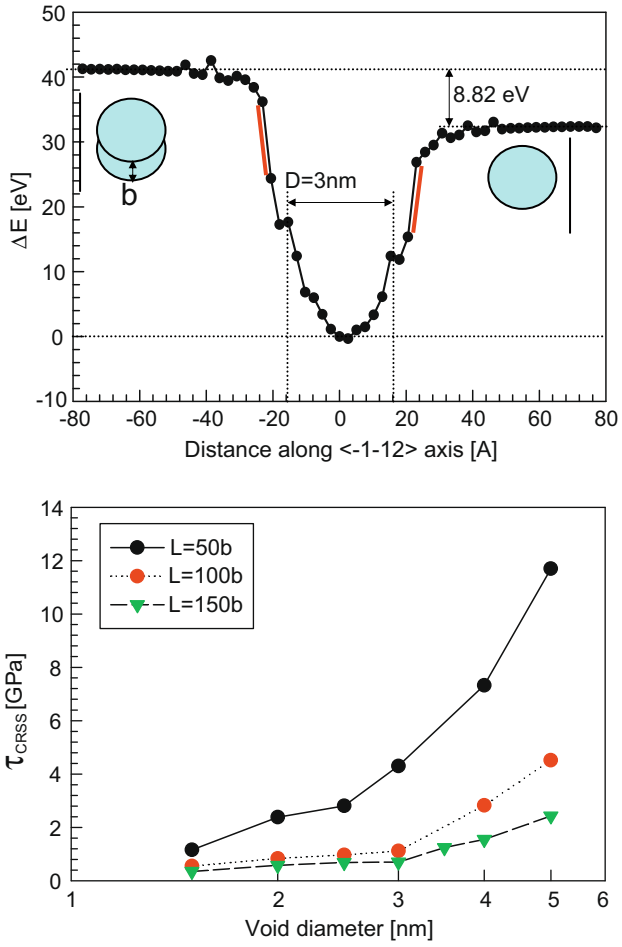


**Fig. 3.** Static simulation results: (a) Excess potential energy as a function of screw dislocation position relative to a 3 nm void centered at the center of the ⟨1 1 2⟩ axis. The asymmetry in the curve at the periodic boundary conditions (distance = ±80 Å) results from introducing a sheared surface step of one Burgers vector on the void following dislocation passage. (b) Critical resolved shear stress ($\tau_{CRSS}$) for a screw dislocation interacting with a regular array of voids, as calculated by Eq. (1) from the conjugate gradient MS calculation results for void diameters between 1.5 and 5.0 nm and inter-particle spacings between 50 and 150 $b$. A significant increase in the $\tau_{CRSS}$ occurs for void sizes larger than about 3 nm in diameter.

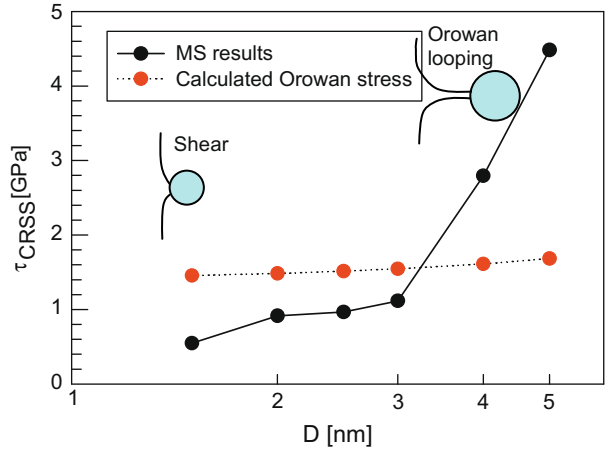


**Fig. 4.** The critical resolved shear stress ($\tau_{CRSS}$) as a function of the void diameter ($D$). The calculated $\tau_{CRSS}$ from the MS results increases abruptly at $D = 3$ nm. The calculated Orowan stress is lower than the MS results at $D > 3$ nm, suggesting a possible change in the interaction and detachment mechanism at $D \sim 3$ nm.

screw dislocation motion. The similar interaction behavior between a void and a screw dislocation is observed even at higher temperature ($T = 1000$ K), where the dislocation glides on {1 1 2} plane. In summary, the screw dislocation interaction and detachment with void occurs via a shear mechanism and the void is sheared by one Burgers vector as a result of each passage of the dislocation in MD simulations.

Thus, the preliminary MD simulation results have not demonstrated a change in the dislocation–void interaction mechanism from shear to Orowan looping for voids larger than 3 nm diameter, contrary to the predictions of the MS results. The large increase in critical resolved shear stress for void diameters above about 3 nm are not fully understood at this time, and will be further investigated by atomistic simulations.

## 4. Conclusions

Using large-scale MD simulations, we have found that the gliding plane of a screw dislocation in BCC Mo changes from {1 1 0} to {1 1 2} at $T \sim 250$ K as the temperature increases. As well, a smooth to rough transition is observed with increasing applied shear stress, independent of the temperature. When the applied shear stress is further increased, dislocation multiplication is observed in the lower temperature, {1 1 0} glide regime, while nano-twin formation is observed in the higher temperature, {1 1 2} glide regime. The MD results indicate that the screw dislocation interaction with voids of diameter from 1.5 to 5 nm occurred via a simple shear mechanism independent of void size. However, the obstacle strength calculated from MS calculations shows a large increase in critical resolved shear stress for void diameter larger than about 3 nm, indicating a possible change in the interaction mechanism. Currently, detailed dynamic studies on the interaction mechanism between a screw dislocation and void as a function of the void size are in progress. Other ongoing research activities include MD and MS simulations of screw dislocation interaction with vacancy and self-interstitial type dislocation loops, as a function of loop Burgers vector and interaction geometry.

## Acknowledgements

We gratefully acknowledge the financial support of the Office of Fusion Energy Sciences, US Department of Energy, under Grant DE-FG02-04ER54750, and by the DOE-Nuclear Engineering Education Research (NEER) program under Contract No. DE-FG07-04ID14594.

## References

[1] J. Marian, W. Cai, V. V Bulatov, Nat. Mater. 3 (2004) 158.
[2] S. Liu, J. Moteff, R.W. Hendricks, J.S. Lin, J. Appl. Crystallogr. 11 (1978) 597.
[3] R.O. Scattergood, D.J. Bacon, Acta Metall. 30 (1982) 1665.
[4] T.D. de la Rubia, M.W. Guinan, J. Nucl. Mater. 174 (1990) 151.
[5] M.W. Finnis, J.E. Sinclair, Philos. Mag. A 50 (1984) 45.
[6] C. Woodward, S.I. Rao, Phys. Rev. Lett. 88 (2002) 216402.
[7] S. L Frederiksen, K.W. Jacobsen, Philos. Mag. 83 (2003) 365.
[8] J. Li, C.Z. Wang, J.P. Chang, et al., Phys. Rev. B 70 (2004) 104113.
[9] F. Shimizu, S. Ogata, H. Kimizuka, et al., J. Earth Simulat. 7 (2007) 17.
[10] V. Vitek, Philos. Mag. 84 (2004) 415.
[11] G. Wang et al., J. Comput.-Aid. Mater. Des. 8 (2001) 117.
[12] J. Chaussidon, M. Fivel, D. Rodney, Acta Mater. 54 (2006) 3407.
[13] J.W. Martin, Micromechanisms in Particle-Hardened Alloys, Cambridge University Press, Cambridge, 1980.
[14] T. Hatano, H. Matsui, Phys. Rev. B 72 (2005) 094105.
[15] Y.N. Osetsky, D.J. Bacon, Philos. Mag. 83 (2003) 3623.