Journal of Nuclear Materials 386–388 (2009) 64–66

Contents lists available at ScienceDirect

Journal of Nuclear Materials

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

3D Dislocation dynamics modelling of interactions between prismatic loops and mobile dislocations in pure iron

Roman Novokshanov *, Steve Roberts

Department of Materials, University of Oxford, Oxford, UK

A B S T R A C T

3D Dislocation dynamics simulations have been carried out to model the interaction between prismatic loops and dislocations in pure iron subject to uniaxial loading conditions. The primary goal was to understand the mechanism of interaction of an $a/2$ <1 1 1> interstitial loop and a mobile dislocation. The secondary goal was to investigate the dependence of the critical stress needed for dislocations to overcome the obstacles as a function of size of loops and their orientation with respect to the glide plane. The simulations have shown a complicated 3D interaction resulting in the mobile dislocation bowing around a loop, either reacting with the loop dislocation or leaving it behind unchanged.

1. Introduction

Neutron irradiation can increase the yield stress and reduce the ductility of metals. These effects are mainly caused by the interaction of dislocations with damage produced during irradiation. In iron irradiated with fast neutrons the damage takes the form of ½ <1 1 1> and ½ <1 0 0> prismatic dislocation loops. The interaction between ½ <1 1 1> loops and edge dislocations is the subject of this research.

The MicroMegas dislocation dynamics (DD) framework was used. The algorithm implementation is based on the lattice method and operates with edge, screw and mixed types of dislocation segments. The total force acting on each dislocation segment is calculated and a mobility law is used to get a position of the segment for the next time step. A set of rules are implemented to take into account the restrictions imposed on dislocation mobility due to the crystal structure of the material been modelled. The model allows cross-slip of screw dislocations. The MicroMegas code is developed and maintained at LEM-ONERA, Paris. More detailed information can be found in [1,2].

2. Mobility law

The following mobility law was used for edge, screw and mixed dislocation segments:

$$v = v_0 \left(\frac{\tau}{\tau_0}\right)^m \exp\left(-\frac{E_a}{kT}\right),$$

where the functions $m(T)$, $V_0(T)$, $\tau_0(T)$, $E_a(T)$ are third-order polynomials depending on temperature and were fitted to the limited data for edge dislocation velocities in iron [3]

$$\begin{aligned}
m(T) &= 12.9 - 6.15 \cdot 10^{-2} T + 9.85 \cdot 10^{-5} T^2 - 1.29 \cdot 10^{-8} T^3, \\
v_0(T) &= 2.75 - 3.06 \cdot 10^{-2} T + 1.16 \cdot 10^{-4} T^2 - 1.43 \cdot 10^{-7} T^3, \\
\tau_0(T) &= 4.04 - 3.12 \cdot 10^{-2} T + 1.50 \cdot 10^{-4} T^2 - 2.34 \cdot 10^{-7} T^3, \\
E_a(T) &= 0.073 + 3.24 \cdot 10^{-3} T - 1.15 \cdot 10^{-5} T^2 + 1.12 \cdot 10^{-8} T^3.
\end{aligned}$$

The polynomial representations of these functions give an extremely good fit to experimental data for dislocation velocity inside the temperature interval from 77 K to 373 K. The dependence of activation energy on temperature, similar to that used here, was discussed in [4]. Very little data are available for screw dislocation mobility in iron. In [5] the screw dislocation velocity in pure iron was measured to be less than half that of edge dislocations at high stresses, where the velocity range was 1–10^3 ms^{-1}. For the lower stresses prevalent in the simulations reported here, the difference between edge and screw velocities is likely to be larger. To reflect this, in the present paper the velocity for screw segments has been taken as 0.1 of the velocity for edge and mixed segments, by setting v_0(screw, mixed) = 0.1 v_0(edge).

3. Cross-slip mechanism

The cross-slip rules implemented were based on the Friedel–Escaig cross-slip model [1]. The probability of the cross-slip is calculated as

$$P = A \exp\left(-\frac{(\tau^* - \tau)V}{kT}\right),$$

* Corresponding author.
E-mail address: novoksha@maths.ox.ac.uk (R. Novokshanov).

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doi:10.1016/j.jnucmat.2008.12.060

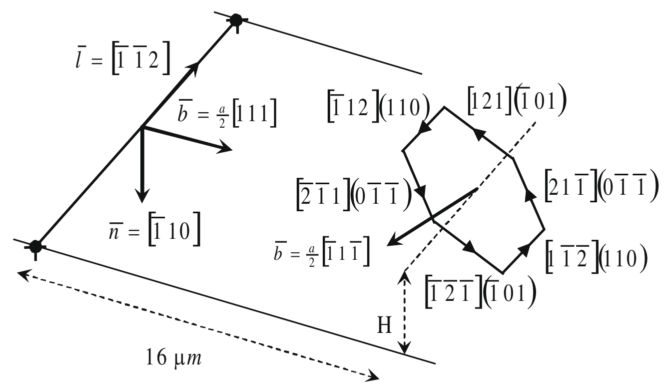

Fig. 1. The configuration modelled; an inclined interstitial prismatic loop ($b = a/2$ $[\bar{1}1\bar{1}]$) and a mobile dislocation ($b = a/2$ [111]). The line directions and the slip planes of the segments forming the loops are shown.

where A is a normalization factor, V is an activation volume, τ^* is the critical resolved shear stress on the cross-slip plane required for formation of the critical cross-slip configuration, and τ is the effective resolved shear stress on the cross-slip plane. For iron $V = 20b^3$ was used [6,7]. A Monte-Carlo method is used to calculate whether cross-slip happens and which cross-slip plane is involved [1,2]. The normalization factor A was set to give a cross-slip probability equal to 1 for a test problem with two screw segments having opposite Burgers vectors placed onto parallel slip planes separated by 50 nm. This is the smallest spacing of stable screw dislocation dipoles in copper deformed cyclically at room temperature with the critical stress about 15 MPa as described in [8]. Since there is no such data available for iron, the same separation value was taken for the simulations presented in this paper. In [9] the critical stress versus screw dislocation length was calculated; the stress rapidly decreased to a stationary value with increasing dislocation length. Based on these calculations the critical stress $\tau^* = 60$ MPa was used in the model, independent of screw dislocation length.

4. Mobile dislocations interacting with a row of inclined prismatic loops

The configuration under consideration is shown in Fig. 1. The box size was 100 μm × 100 μm × 100 μm with periodic boundary conditions, the temperature modelled was 300 K, the strain rate was $2 \cdot 10^{-4}$ s^{-1} and the loading direction was [100]. The interaction of a mobile edge dislocation with a row of $a/2$ $[\bar{1}1\bar{1}]$ prismatic loops, each separated by one loop diameter, was modelled. Each prismatic loop was modelled as six connected pure edge segments with $b = a/2$ $[\bar{1}1\bar{1}]$ on $(\bar{1}10)$, $(\bar{1}01)$ and $(0\bar{1}1)$ slip planes. A Frank-Read source consisting of a pure edge segment with the Burgers vector $a/2$ [111] and the line direction $[\bar{1}\bar{1}2]$ was placed onto the $(\bar{1}10)$ plane. The original length of the source was 4 μm and its separation from the row of loops was 16 μm. The separation H between the source gliding plane and the row of loops was varied over a wide range.

In these simulations, because of limitations of stability of the DD code used, the loops simulated were of diameters starting with 80 nm. This is larger than loop sizes observed by TEM in iron as a result of low-temperature neutron irradiation (e.g. [10]) but is within the size range of loops observed to be produced by self-ion irradiation at higher temperatures (300–500 °C) [11]. However, because the modelling uses a continuum method based on purely elastic interactions, the results should not vary appreciably with

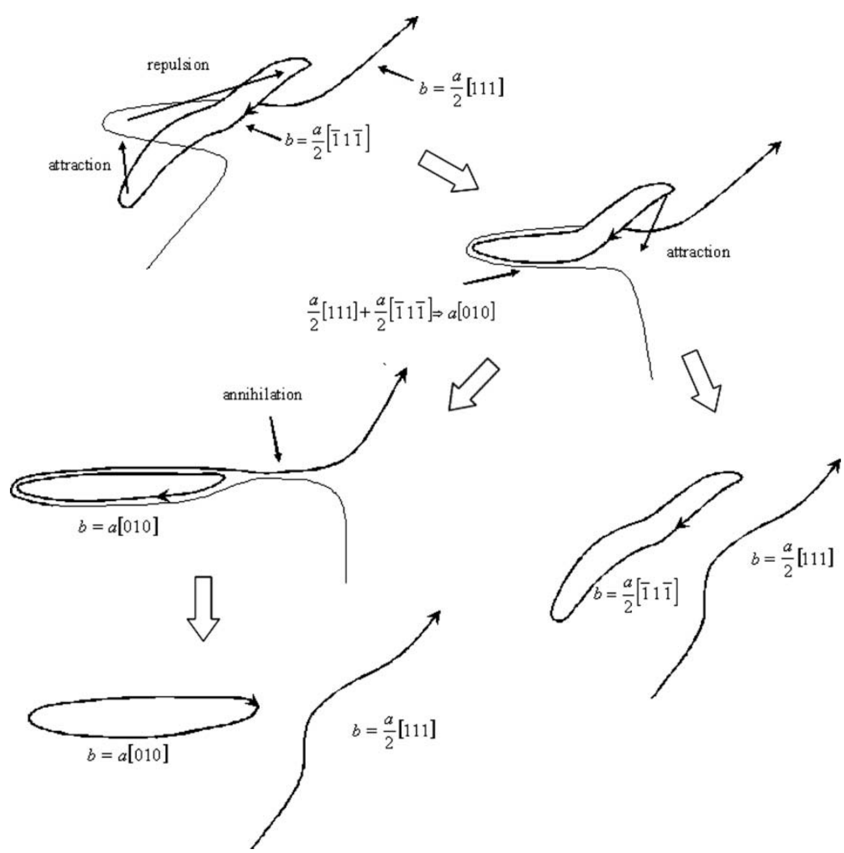

Fig. 2. The two observed mechanisms of interaction of a prismatic loop with a dislocation gliding along an inclined plane.

scale, provided the ration between loop size and loop spacing is kept constant, as here. It is possible that reactions involving dislocation climb, which are not included in this DD implementation, might cause the results to differ from those actually operating at very small loop sizes; here, comparison between the mechanics of interactions predicted by DD and by MD will be of interest.

When H is larger than the radius of a loop, the strength of the interaction was found to rapidly decrease with increasing H. In the case when H is less than the radius of a loop the simulations reveal two possible scenarios, shown in Fig. 2. Initially the gliding dislocation emitted from the source feels repulsion from the top and attraction from the bottom of the loop ('top' and 'bottom' are for the particular senses of b used for the loop and mobile dislocations). After the bottom part of the loop has been attracted into the glide plane of the Frank-Read source the mobile dislocation continues bowing around the loop. Here the balance of repulsive and attractive forces becomes more important. If the attraction forces prevail over the repulsion forces, the upper part of the loop is attracted by the other parts of the mobile dislocation finally producing a trapped loop around the original prismatic loop which becomes rotated. The pair of superimposed dislocation lines corresponds to the reaction:

$$\frac{a}{2}[1\,1\,1] + \frac{a}{2}[\bar{1}\,1\,\bar{1}] \Rightarrow a[0\,1\,0].$$

On the other hand if the attraction forces are not strong, the mobile dislocation unlocks from the loop. The simulations have shown that the locking mechanism is more likely to happen when $H \sim 0$ so that the mobile dislocation goes close to the centre of loops, otherwise the unlocking mechanism is more likely to occur.

For all interactions of the mobile dislocation with the loops the critical stresses τ_{loc} were calculated according to

$$\tau_{loc} = \frac{Gb}{L}\cos\varphi_c,$$

where G = 89 GPa is the shear modulus, b = 0.248 nm is the Burgers vector, L is the average separation between loops and ϕ_c is the measured critical angle. The critical stresses are shown in Fig. 3. The maximum stress observed is about 220 MPa for all loops in the size range D = 80–100 nm. The critical stress reported in [12] determined for loops of size 5 nm in iron using molecular dynamics simulations is 212–220 MPa, close to that obtained by the dislocation dynamics simulations presented here. This is interesting, as the implication is that the strength of the loop – mobile dislocation interactions is dominated by the elastic interactions present in both the MD and the DD simulations, rather than by the non-conservative aspects of dislocation motion which are included only in the MD simulations.

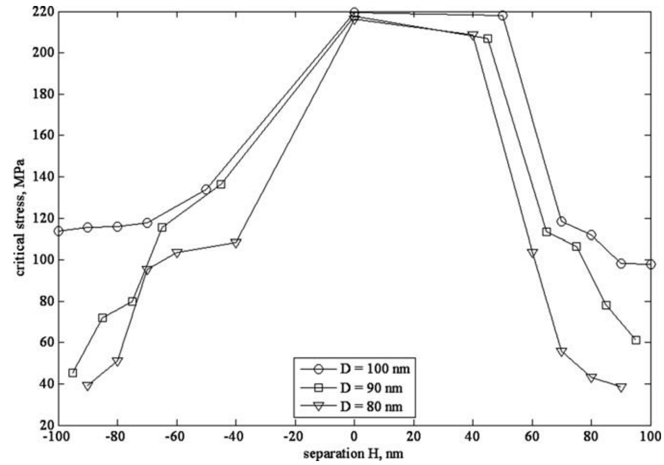

Fig. 3. Critical stresses the mobile dislocation to pass the row of prismatic loops of three diameters D (80 nm, 90 nm, 100 nm), as a function of the initial 'vertical' separation H between the dislocation glide plane and the row of loops.

Acknowledgements

The support of this research by the EPSRC, under grant GR/S81155 is gratefully acknowledged. We also acknowledge useful discussions with Professor Sergei Dudarev and Professor David Bacon.

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