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# 3D dislocation dynamics study of plastic instability in irradiated copper

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**Abstract**

The onset of plastic instability in neutron irradiated copper is investigated by computer simulation of the dynamics of the elastic interaction between dislocation loops emitted from Frank–Read (F–R) sources and irradiation-induced defect clusters. We show that small prismatic defect clusters produced directly from collision cascades are trapped in the stress field of slip dislocations, and that mobile clusters are absorbed in the dislocation core, when they approach within ~6 nm. Sessile vacancy clusters are also absorbed within this 'stand-off' distance because of an induced surface tension on their stacking fault. The interaction between prismatic defect clusters in 'decorations' and dislocations is shown to provide significant resistance to the initiation of plastic deformation in irradiated copper (source hardening). Sessile stacking fault tetrahedra are also shown to resist dislocation motion by localized forces before they are absorbed and removed by activated dislocation sources. The significance of these mechanisms to initiation of localized deformation and plastic instability are discussed. 

## 1. Introduction

Experimental results consistently show that neutron irradiation of metals and alloys at temperatures below recovery stage V causes substantial increase in the upper yield stress and induces yield drop and plastic instability. Commonly, irradiated metals exhibit yield drop (following the upper yield point), do not show any work hardening and in many cases even show work softening. This specific type of plastic flow localization is considered to be one of many possibilities of plastic instabilities treated in the literature [1]. At the upper yield point, plastic deformation is likely to be initiated in a localized fashion at sites acting as dislocation sources in the form of slip bands. These sites could be the locked dislocations themselves or where the applied stress is intensified (e.g., grain boundaries, inclusions, triple points, etc.). High velocity dislocations thus generated at sources may cut through soft and incoherent precipitates, or destroy previously built-up dislocation structures [2,3], causing softening in the active slip plane.

Following neutron irradiation, yield drop is observed to occur in pure fcc, bcc and hcp metals and alloys, provided that they are irradiated and tested at temperatures below recovery stage V [4–6]. Recently, it has been proposed that the phenomenon of yield drop is caused by decoration of grown-in dislocations by small clusters or loops of self-interstitial atoms (SIAs) produced in displacement cascades [4–6]. Consequently, dislocations are immobilized, in a manner similar to that in the case of dislocations with an 'atmosphere' of impurities or solute atoms in un-irradiated iron [7] or Cu–30% Zn alloy [8]. It has been shown that the decoration of dislocations by small SIA clusters is likely to occur, but only under cascade damage conditions where small glissile clusters are produced in displacement cascades [5,6].

Investigations of post-deformation microstructure of irradiated metals and alloys have provided evidence for the formation of 'cleared' channels (see [3,5,9] for reviews). In the volume between these channels no mobile

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dislocations are created during deformation. Once fresh dislocations are generated, they move very fast on their glide planes and cut, absorb or sweep irradiation-induced defect clusters and loops present on the glide plane [10–12]. Consequently, cleared channels become almost defect free and thereby soft material for dislocation transport. This reinforces plastic strain localization and induces instability in plastic flow.

To explain experimentally observed hardening behavior, a new model called cascade induced source hardening (CISH) was developed [4–6]. Grown-in dislocations are decorated by small sessile clusters of SIAs produced in the cascades. The CISH model is used to calculate the stress necessary to pull the decorated dislocations from the atmosphere of defects around them so that they can act as dislocation sources. The stress thus calculated is taken to represent the upper yield stress. Fig. 1 shows experimental results for irradiation-induced increase in the upper yield stress and the occurrence of yield drop in pure copper and pure iron irradiated with fission neutrons at $\sim$320 K. It can be observed that irradiated copper and iron are not able to work-harden after the yield drop.

In this paper, we present results of recent 3D dislocation dynamics calculations of the external stresses necessary to drive dislocation loops generated from a Frank–Read (F–R) source, through a random field of small SIA loops or SFTs on its glide plane. The stress necessary to unlock the dislocation from non-coplanar

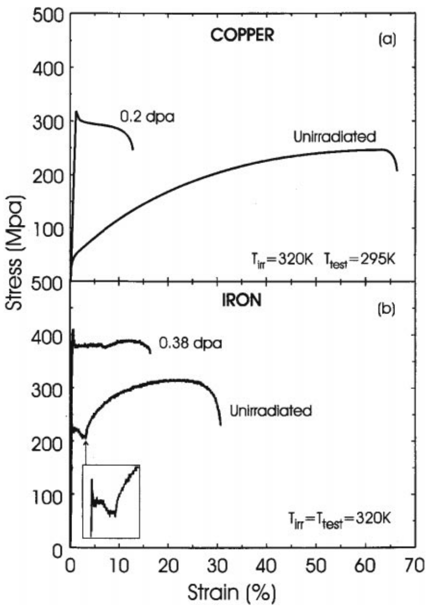


Fig. 1. Stress–strain curves for irradiated and un-irradiated Cu and Fe. Both Cu and Fe specimens were irradiated in DR-3 reactor at RISO at 320 K, and tensile tested at 295 and 320 K, respectively.

defect decorations is also calculated. A brief outline of the theoretical basis for computer simulations is given next in Section 2, followed by results of numerical computer simulations in Section 3. Finally, conclusions of the study are presented in Section 4.

## 2. Method of computer simulation

Ghoniem and his co-workers [13–15] have recently developed the method of parametric 3D dislocation dynamics for computer simulations of mesoscopic plastic deformation. The application of this method to the problem of dislocation decoration with defect clusters is explained in [16]. In this approach, we first rewrite Burgers displacement equation for a loop in index tensor form. The displacement vector is then differentiated to obtain the elastic strain in an isotropic material as a line integral. The stress tensor is computed from the linear relationship between the strain and stress, which is then discretized by parametric segments, and the total stress field computed by numerical quadrature. The geometry of dislocation segments is represented in parametric vector form as: $\hat{\mathbf{r}}^{(j)}(u) = \sum_i \mathbf{q}_i^{(j)} N_i(u)$, , where the vector $\hat{\mathbf{r}}^{(j)}(u)$ represents the spatial position of segment ($j$). A set of parametric shape functions $N_i(u)$, and generalized coordinates $\mathbf{q}_i^{(j)}$ completely determine the shape of the segment. The degrees of freedom (i.e., generalized coordinates) are the displacement, tangent and normal vectors at each nodal position. The stress tensor $\sigma_{ij}$, and the interaction energy between two loops, $E_{\mathrm{I}}$, can be obtained as fast numerical sums over the number of quadrature points $Q_{\max}$ on each segment, the loop segments $N_{\mathrm{s}}$, and the number of loops $N_{\mathrm{loop}}$ in the simulation volume. The total force acting on defect clusters is [18]: $F_i = -n_j \sigma_{jk,i} b_k \delta A$, while the torque, which attempts to rotate the cluster is: $M_i = -\epsilon_{ijk} n_j \sigma_{lk} b_l \delta A$. $\epsilon_{ijk}$ is the permutation tensor, $n_j, \sigma_{lk}$ and $b_l$ are the Cartesian components of the habit plane normal, the stress tensor, and the Burgers vector, respectively, and $\delta A$ is the cluster area. As the defect cluster moves closer to the core of the slip loop, the turning moment on its habit plane increases. If the amount of mechanical work of rotation exceeds a critical value (0.1 eV/crowdion [16]), then it is assumed to change its Burgers vector and habit plane, and move to be incorporated into the dislocation core. The critical surface for cluster rotation and hence subsequent absorption into the dislocation core has been determined [16]. The large local stress field close to the dislocation loop core can result in an *induced surface tension* on the loop [16]. The induced surface tension is given by the additional work done in expanding the surface area of the loop in the existing field: $\gamma = n_i \sigma_{ij} b_j$. Since the stress field and cluster orientation are both involved in determining the induced surface tension, the energy value can be either positive or negative. Thus, the critical unfaulting radius for a typical dislocation cluster may increase or decrease from its unstressed value, depending on whether the additional virtual work adds or subtracts from the stacking fault energy.

The equations of motion for dislocation segments arew derived from a Galerkin minimum energy principle. The position, tangent and normal vectors of nodes on continuous dislocation lines are updated at every time step. The stress field is used to calculate the Peach–Kohler force components of all surrounding defect clusters on any slip loop. Self-forces are computed from the slip loop geometry (local curvature), while the applied stress and the Peierls lattice friction stresses are added to the internal and self-forces at each node. The dislocation velocity $\vec{v}$ is related to the net force $\vec{F}$ on the dislocation segment as: $\vec{v} = M\vec{F}$, where $M$ is the dislocation mobility [14,15].

## 3. Results

In Cu, hexagonal faulted Frank loops of type $\frac{a}{3}\langle 1\,1\,1\rangle$ $\{1\,1\,1\}$ are found to be stable and sessile, while very small loops (containing only tens of interstitials), with $\mathbf{b} = \frac{a}{2}\langle 1\,1\,0\rangle$ are glissile. Sessile vacancy clusters in Cu are $\{1\,1\,1\}$-platelets of stacking fault tetrahedra (SFTs) [19]. We consider here a three-step procedure to determine the magnitude of radiation hardening and subsequent work softening in dislocation channels beyond the upper yield point: (1) 'decoration' of dislocations with defect clusters during irradiation; (2) the onset of plastic yield (upper yield point) as a result of unlocking dislocations from non-coplanar sessile clusters in the decoration zone at highly-stressed regions of the crystal; (3) plastic softening resulting from cluster resistance (mainly SFTs) and destruction by subsequent dislocation motion on the glide plane. We give here a summary of the main results of calculations for the first two steps, followed by more details of dislocation 'clearing' of channels by destruction of SFTs.

### 3.1. Dislocation decoration with defect clusters

The interaction energy between dislocations and defect clusters has been calculated to estimate: (a) the minimum 'stand-off' distance between clusters and dislocations; (b) the 'unfaulting' zone for sessile Frank loops. Our calculations [16] indicate that the trapping, or 'capture' distance in Cu is on the order of 18 nm at room temperature. As a result of an induced torque on interstitial clusters, they tend to change their Burgers vector and rotate to be absorbed at a critical stand-off distance of ∼9 nm. For sessile Frank loops, the stress-free unfaulting radius of ∼22 nm is found to be dramatically altered near the core of the slip loop. On the compressive side, the stress field shrinks the critical unfaulting radius to ∼6 nm, while it expands significantly on the tensile side. It is estimated that small SFTs will unfault and get absorbed into the dislocation core at a distance of ∼6 nm. When the dislocation approaches an SFT on its glide plane, it may collapse into a Frank loop and then get absorbed in the dislocation core. The SFT is therefore assumed to be a weak obstacle to dislocation glide, and it is totally destroyed upon passage of the first dislocation loop.

### 3.2. Dislocation unlocking from defect clusters at the upper yield point

As the loop expands, each point on the dislocation line will experience a resistive (or attractive) elastic force from defect clusters. In addition, the loop line curvature will also change, and will require additional applied stresses to allow its continued expansion. When the applied stress plus the local self-stress resulting from bending around the cluster attain a critical value, the dislocation to breaks free (unlock) from the elastic field of the cluster. In our calculations [17] for the interaction dynamics between a single cluster at the stand-off distance away from the glide plane and an expanding dislocation loop, the time step is dynamically determined (it is in the range 5 ps to 0.1 ns). It is found that the dislocation line is first 'pinched-off' at its distance of closest approach to the cluster, and thus must change the sign of its curvature. Once the curvature changes, the local value of the dislocation self-force becomes great enough to assist the applied stress in overcoming the resistance of the cluster to dislocation motion. The resistance force field of clusters is stochastic, and is punctuated by high force values for clusters that reside close to the stand-off distance. The force per unit length imposed by clusters on the dislocation is found to be as high as ∼200 (MPa $\times\, a$), where $a$ is the lattice constant. This high force value corresponds to the upper yield point. The exact value of the upper yield point is found to be sensitive to the cluster density near decorated dislocations at the stand-off distance.

### 3.3. Plastic softening beyond the yield point

Following dislocation unlocking events from surrounding atmospheres, they interact with sessile obstacles on the glide plane. In irradiated copper, these obstacles are SFTs or sessile faulted vacancy loops. Based on simple energy estimates [16], we assume that SFTs unfault as a result of the interaction with the stress field of passing dislocations. SFTs will offer resistance to dislocation motion by short-range interactions, and they can be overcome once the local force on the interacting dislocation segment exceeds the intrinsic strength of the obstacle, as described by the critical angle to destroy the obstacle ($\phi_C$). Results of computer simulations for

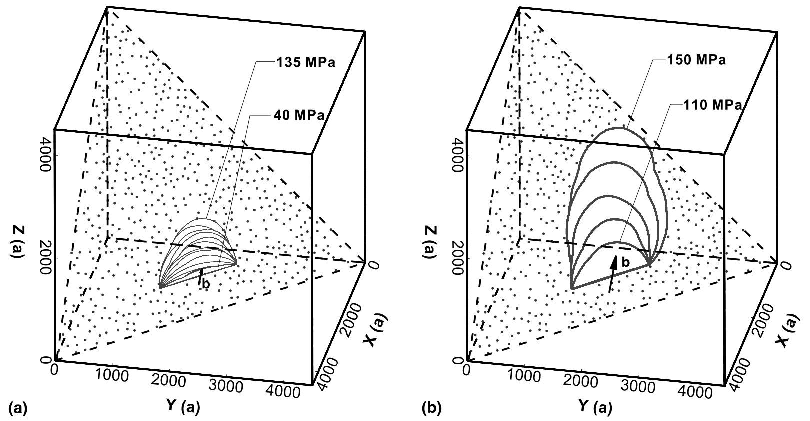


Fig. 2. Computer simulations of the early stages of plastic slip emanating from a single F–R source in copper irradiated and tested at 100°C. Displacement damage dose = 0.001 dpa, STF's density = $1.0 \times 10^{23}$ m$^{-3}$, size = 2.5 nm. Simulated crystal size = 4500$a$ (~1.62 μm). Initial F–R source length = 1600$a$ (~576 nm). Stress is applied along [1 0 0]–$\sigma_{xx}$.

the early stages of plastic slip propagation (emanating from a single F–R source) in copper irradiated and tested at 100°C and 0.001 dpa is shown in Fig. 2(a). A tensile stress ($\sigma_{xx}$) is applied along [1 0 0]-direction, and is gradually increased. At each stress step, the equilibrium loop configuration is computed, and when the angle between the tangent vectors at an SFT is reaches its critical value (taken as 160°), the two subtending segments are released and the SFT is destroyed and removed from the simulation. It is observed from Fig. 2(a) that the dislocation loop is sometimes 'stuck' at SFTs till neighboring segments achieve the critical angle condition. Fig. 2(b) shows the results of calculations of loop positions at larger stress steps, as compared to Fig. 2. Note that the dislocation loop is deformed along the general direction of its Burgers vector to minimize its self-energy.

For a single slip plane within the dislocation channel, the applied stress must be incremented gradually thus allowing dislocation loops to assume successive quasi-equilibrium positions. A comparsion between computed and experimental measurements of the flow stress in copper irradiated and tested at 100°C [20] is shown in Fig. 3. The displacement damage dose = 0.01 dpa, STF's density = $2.5 \times 10^{23}$ m$^{-3}$, size = 2.5 nm [20]. The applied stress is plotted against the local strain on the glide plane (ratio of swept to total area). Dislocation motion is seen to be difficult at low applied stresses, till a critical value is achieved (flow stress). At this stress, the dislocation loop will overcome any SFT without an additional increase in the applied stress. The influence of the critical interaction angle between dislocations and SFTs is also shown, and as expected, the smaller the critical angle, the larger the flow stress. Reasonable agreement with experiments is obtained for plastic slip initiation on one single plane. The influence of intra-plane dislocation–dislocation interactions on the flow stress of irradiated copper is shown in Fig. 4. The mutual interaction between two F–R sources in copper irradiated and tested at 100°C in the random field of SFTs results in some additional deformation of the two F–R sources, which are separated by 500$a$ (~180 nm). All other conditions are the same as in Fig. 2. A slightly higher flow stress is required in this case. At smaller separation distances, the mutual interaction of expanding F–R sources can be significant, and the required flow stress is thus correspondingly increased (for more details, see Ref. [17]).

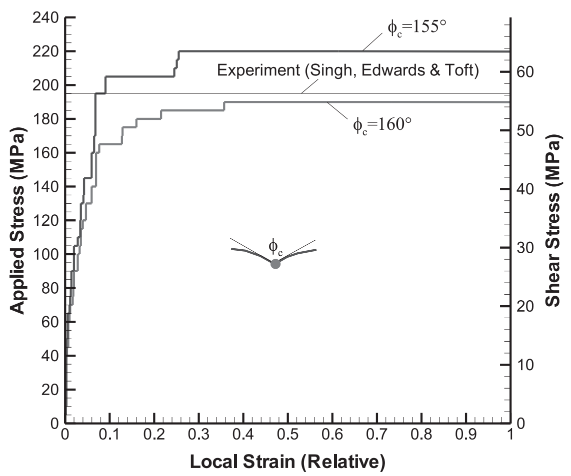


Fig. 3. Comparsion between computed and experimental [20] flow stress in copper irradiated and tested at 100°C. Displacement damage dose = 0.01 dpa, STF's density = $2.5 \times 10^{23}$ m$^{-3}$, size = 2.5 nm. The influence of the critical interaction angle between dislocations and SFTs is also shown.

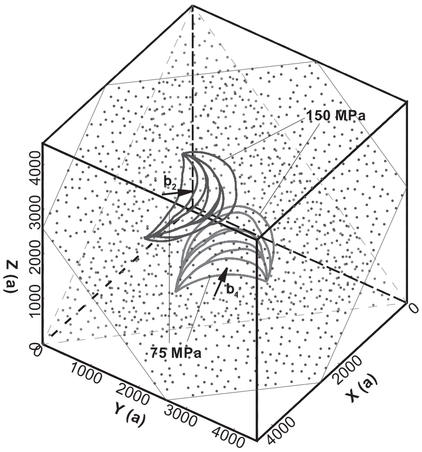


Fig. 4. Propagation of plastic slip emanating from two interacting F–R sources in copper irradiated and tested at 100°C. The two F–R sources are separated by 500$a$ (∼180 nm). Conditions are the same as in Fig. 2.

## 4. Conclusions

Under irradiation, dislocation loops in copper are shown to attract mobile defect clusters. The size of the elastic capture zone is primarily determined by their interaction with the edge components of slip loops. At room temperature, calculated trapping zone sizes are on the order of 18 nm. Clusters which are produced closer than a stand-off distance of ∼6 nm from the dislocation core are absorbed, either due to a high torque on their habit plane or due to unfaulting of small Frank loops. The resistive force per unit length of a decorated dislocation, as a result of its interaction with a single cluster at the stand-off distance is estimated as ∼200 (MPa $\times\, a$) at the point of closest approach. Thus, the magnitude of the 'unlocking stress' for source hardening is dependent on the cluster density within the decorated zone. Most of the contributions to the resistive motion of slip dislocations are produced from nearby clusters close to the stand-off. Once the dislocation is unlocked from its immediate surrounding clusters, it propagates on the slip plane by interaction and absorption of prismatic loops and SFTs. The current results indicate that the magnitude of the flow stress can be reasonably predicted, and that it is in good agreement with experiments on irradiated copper [20]. The mechanism of attaining the 'flow' stress is explained in terms of percolation of dislocation segments through a random field of co-planar SFTs. The predictions are not very sensitive to dislocation–dislocation hardening effects, but are rather determined by the interaction between dislocations and SFTs. The only adjustable parameter in these calculations is the critical angle for dislocations to break-away and destroy SFTs. The current results clearly demonstrate that in calculating the resistance to dislocation motion, the influence of both coplanar and non-coplanar loops and SFTs must be considered. While non-coplanar defect clusters in the decoration zone determine the unlocking stress, coplanar SFTs are responsible for the magnitude of the flow stress. Their removal by unfaulting mechanism appears to be the controlling factor for the occurrence of flow localization and the onset of plastic instability in irradiated copper.

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