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New insights into radiation hardening in face-centered cubic alloys

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In face-centered cubic (fcc) metals, defects with dislocation character are the main component of the radiation microstructure. Despite the large number of reported interaction mechanisms, a significant ratio of interactions results in defect absorption, leading to the forming of superjogs and helical turns. Since absorption is controlled by elastic relaxation, dislocation dynamics simulations are used to determine the corresponding hardening. In agreement with experiments, simulation results reveal a strong hardening level, independent of the alloy friction or the dislocation velocity.

Keywords: Strengthening; Dislocation dynamics; Radiation hardening; Dislocation loops; fcc

The radiation microstructure in face-centered cubic (fcc) alloys is basically formed of dislocation loops (DLs), stacking fault tetrahedrons and unresolved black dots [1]. Since, black dots were recently identified as small DLs [2], most radiation defects thus have a dislocation character. On the other hand, irradiation is known to induce great strengthening [3]. Following the disperse barrier hardening model [4], the average planer spacing l of defects of average size D and number density C is $(DC)^{-1/2}$, and the increase in the critical resolved shear stress $\Delta\tau$ is given by:

$$\Delta\tau = \alpha G b\sqrt{DC} \tag{1}$$

where α is a coefficient accounting for the strength of the defect, G is the shear modulus and b is the norm of the Burgers vector. From fitting experimental results of neutron-irradiated austenitic stainless steels, α was found to be between 0.42 and 0.52 [5,6] and between 0.25 and 0.44 [7], while in nickel it was close to 0.5 [8]. These values are substantially larger than the analytical estimate for randomly distributed loops [9].

Atomistic simulations (ASs) were used to study the interactions between radiation defects and mobile dislocations. ASs have revealed a large number of mechanisms [10,11]. However, it is found that if the defect is not too large (say, a few nanometers) and the dislocation velocity is not too large (say, a few meters per second), most defects are absorbed when they get close to the impinging dislocation, leaving double superjogs on edge dislocations (EDs) [12] and helical turns on screw dislocations (SDs). This was established in nickel [13] and in materials of low and high stacking fault energy [14,15] and confirmed in experiments [16]. The absorption seems to increase with temperature and decrease with stacking fault energy. At a larger simulation scale, Mastorakos and Zbib [17] proposed another formula for radiation hardening in α-iron, fitted on dislocation dynamics (DD) results. DD was also used to investigate dislocation decoration [18,19] and interaction with uniform and segregated loop distributions [20,21] according to the cascade-induced source hardening model [22]. In these papers, the contact reaction with mobile dislocations was not accounted for: defects within a critical distance were explicitly removed from the simulation box, leaving only the possibility of long-range elastic interactions to impede dislocation motion. This is probably at the origin of the low hardening reported with randomly distributed defects. Recently, Arsenlis et al. [23] used DD simulations to investigate interactions with perfect prismatic loops in α-iron. They provided a value of $\alpha = 0.27$, which is close to the strength of forest dislocations. However, the size of the considered loops is quite large compared with typical defect sizes in irradiated materials [1], and non-elastic interaction features, such as the rotation of the loop Burgers vector, were not allowed.

Absorption is thus the predominant interaction result with small loops while, at the same time, its strength is large [14]. This is why it is necessary to correctly estimate the hardening effect of the absorption mechanism. To do this, all loops were taken to be of collinear type, i.e. sharing the same Burgers vector as the mobile dislocation. Because the reaction with collinear dislocation loops (CDLs) is completely controlled by elastic relaxation [24], DD simulations were used to predict dislocation interactions with the CDLs and to determine the induced hardening.

The DD technique used in this work has been described in a separate paper [25]. We present here only the specific

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features peculiar to the present study. An ED or SD is introduced into a rectangular parallelepiped, used to model a small fcc crystal, containing a large number of randomly distributed CDLs. The crystal axes are parallel to the Burgers vector (½ $[\bar{1}10]$), to the $[\bar{1}\bar{1}2]$ direction and to the normal of the slip plane [111]. In order to increase the computing efficiency, the dimension parallel to [111] was reduced to four times the size of the CDLs. Periodic boundary conditions were applied in the three directions, resulting in an infinite SD or ED. The simulation box is loaded with a uniaxial constant strain rate. A dislocation segment is allowed to move in the simulation when the effective stress τ_{eff} is larger than a threshold stress, called the friction stress τ_f. Its velocity is given by $v = b(\tau_{eff} - \tau_f)/B$, where B is the friction coefficient. In our simulations, we considered the values $b = 0.25$ nm, $B = 10^{-4}$ Pa.s, a Poisson's coefficient of 0.33 and a shear modulus G of 84 GPa.

The generated loops are initially of edge character of different sizes (2, 3 or 4 nm) and densities (10^{22}–10^{23} m^{-3}). The size of the simulation box parallel to the dislocation line was equal to at least 10 times the average loop planer spacing l, while the box size parallel to the direction of motion was close to 20 l. In addition to the CDL size and density, the effects of the friction stress (10 and 100 MPa) and the average dislocation velocity (1.0 and 0.1 m s^{-1}) were also investigated.

In the case of the ED, simulations reveal a global drag of the CDLs in the direction of motion of the dislocation. When the ED does not cut a CDL in the middle, a net attractive or repulsive force appears. In the repulsive case, the CDL is pushed in front of the edge dislocation, while in the attractive case two configurations can be met. If the CDL cuts the slip plane, a collinear interaction occurs, leading finally to the formation of two superjogs. The initial CDL is truncated, resulting in a CDL of smaller size. When the CDL does not cut the slip plane, it is simply dragged behind the ED. Figure 1(a) shows a snapshot of the ED interacting with 4 nm loops of 2×10^{22} m^{-3} density. It can be clearly observed that many CDLs are gathered in front of the dislocation, while a small density of smaller loops are left behind.

For the SD, Figure 1(b) shows interaction with 2 nm loops of a density equal to 10^{23} m^{-3}. A large density of helical turns with a large bow-out between them can be seen. The density of CDLs is almost the same in front and behind the dislocation. These features are consistent with the interaction dynamics reported by Arsenlis et al. [23]. The loading curves corresponding to these simulations are plotted in Figure 2. Since τ_f was modified in some simulations, the quantity of interest is $\Delta\tau = (\tau_{app} - \tau_f)$, with τ_{app} the applied shear stress. For the sake of brevity, $\Delta\tau$ is called "stress" in the following. In Figure 2, the stress is plotted as a function of the area swept by the dislocation, normalized by the average area per CDL. This allows us to analyze the stress as a function of the number of CDLs swept by the dislocation.

In the ED case, the stress first increases before reaching a plateau with multiple peaks related to pinning–unpinning events. The initial increase can be explained by the loop drag, since every dragged CDL generates a friction force amounting to $4bD\tau_f$. The plateau regime is found to correspond to saturation in the number of dragged CDLs. During the ED motion, the concentration of the dragged loops fluctuates along the dislocation line. The ED starts to bow-out between regions of high CDL density and form segments of screw character. Helical turns then start to form, strongly pinning the curved ED. As can be seen in Figure 2, the plateau is reached rapidly for large CDL density, large friction stress and large dislocation velocity. For $C = 10^{22}$ m^{-3}, $\tau_f = 100$ MPa and $v = 0.1$ m s^{-1}, the plateau is reached after interaction with almost 120 CDLs, while it is reached after interaction with approximately 60 loops for $C = 10^{23}$ m^{-3}, $\tau_f = 10$ MPa and $v = 1$ m s^{-1}. However, the value of the plateau stress seems to be independent of loop size, friction stress or dislocation velocity.

For the SD and after interaction with fewer than 20 CDLs, a stress plateau is reached, basically depending on the CDL density and size, as can be observed on Figure 2. In order to perform a quantitative analysis, we associate with every plateau a single stress value corresponding to the average of stress maxima. This value is thought to be representative of the critical stress, because the magnitude of the stress drop after unpinning mainly depends on the box height, while a stress maximum represents the strength of the loop configuration along the dislocation line. The obtained stress values are plotted in Figure 3 as a function of the CDL density and size, for different friction stresses and dislocation velocities. Data for the SD are indicated by "sc" and those for the ED by "ed". Since CDLs are randomly distributed, we first compare our results with the strengthening induced by impenetrable obstacles, predicted by the Bacon, Kockes and Scattergood (BKS) model reported in Ref. [26] and confirmed later by DD simulations [27]. The stress predicted by the BKS model is given by:

$$\Delta\tau_{BKS} = \left(\frac{\ln \underline{D}}{\ln \underline{l}}\right)^{\frac{3}{2}} \frac{G}{\pi \underline{l}} \ln \underline{l} \tag{2}$$

Here, we note that, in the original paper [20], the authors normalized lengths l and D by b and ignored the constant (0.7) found in the fitting procedure. Since 0.7 is close to ln 2, we believe that normalization must be done by $b/2$. This modification is found to greatly improve the model predictions of the Orowan hardening.

Predictions of Eq. (2) are depicted in Figure 3. The figure shows that the strengthening induced by CDLs is almost twice the strengthening induced by impenetrable particles of the same size and density. The reason is clearly related to the elastic relaxation of the helical turns, which decreases the length of free dislocation segments, as suggested by Rodney [13].

Values of the plateau stress obtained with the ED are also shown in Figure 3. The two dislocations exhibit comparable interaction strengths.

The last analysis of our results is the comparison with experimental results fitted on Eq. (1), which is still widely used in the scientific community. We thus plot in Figure 4 the strengthening obtained in DD simulations as a function of the Orowan stress $Gb\sqrt{DC}$ for different densities, sizes, friction stresses and dislocation velocities. A reasonable linear correlation is obtained, with a slope close to 0.5. This result suggests that the interaction coefficient α in Eq. (1) equals 0.5.

While the effect of the dislocation velocity is negligible (see Fig. 4), the strengthening seems to decrease slightly with increasing friction stress. The relaxation of the helical turn, considered to be at the origin of strengthening, is thus impeded by the friction stress. This effect is thus similar to that observed in forest hardening [28] and confirmed