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Evolution of nanoscale interstitial dislocation loops under coupling effect of stress and temperature

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ABSTRACT

The properties of nano-scale interstitial dislocation loops under the coupling effect of stress and temperature are studied using atomistic simulation methods and experiments. The decomposition of a loop by the emission of smaller loops is identified as one of the major mechanisms to release the localized stress induced by the coupling effect, which is validated by the TEM observations. The classical conservation law of Burgers vector cannot be applied during such decomposition process. The dislocation network is formed from the decomposed loops, which may initiate the irradiation creep much earlier than expected through the mechanism of climb-controlled glide of dislocations.

When materials are operated under the irradiation environment, the formations of self-interstitial atoms (SIAs), SIA-clusters and SIA-loops induced by the interaction between high energy particles and atoms in materials are found to play an important role in understanding different radiation damage processes [1–11]. Under irradiation, the clustering and growth of supersaturated SIAs form SIA dislocation loops, which can be observed by transmission electron microscopy (TEM) when its size reaches to nano-scale. In BCC iron, two Burgers vectors of these loops are confirmed: 1/2 ⟨111⟩ and ⟨100⟩, with different properties [4,6,7,9,10], which are usually explored without considering the stress or strain effect. However, under irradiation (e.g. creep condition), both temperature and stress affect the evolution of dislocation loop in a coupled way, which has not fully studied until now. Recently, the TEM observation of the in-situ ion irradiation has been widely used to understand the radiation damage [9]. By analyzing such experimental process [9], we notice that the high energy in-situ irradiation can result in not only the temperature effect but also the possible thermal-stress effect on existed loops in nano-thick TEM samples. The possible free surface effect induced by nano-thick TEM samples may also affect the evolution of loop. Hence, the evolution of dislocation loops is affected by a coupling condition of stress and temperature. Except such external stress, the high density of the extended defects (e.g. helium bubbles, precipitates) produced by irradiation would also induce high local stress in materials, which may influence the state of dislocation loops. As one of the extended defects, the state change of SIA dislocation loops under the coupling condition is supposed to influence the mechanical properties of irradiated samples. Thus, all these results lead us to address the following questions: (1) how does the coupling condition of stress and temperature influence the properties of nano-scale dislocation loops in irradiated materials and (2) what is the detail of the structural evolution under such coupling effect?

Without stress effect, the stable defect configuration of a single interstitial is a ⟨110⟩ dumbbell in BCC iron [12–14], different from the ⟨111⟩ crowdion in other BCC metals [15]. When the ⟨110⟩ dumbbell is affected by external stress field, e.g. from helium-vacancy cluster, it can transfer to the ⟨111⟩ crowdion with a low energy barrier (0.3–0.4 eV) [16]. Recent calculation shows the formation energy of simple defects (e.g. dumbbell and crowdion) in BCC iron and tungsten is also affected by external hydrostatic strain and uniaxial strain along the ⟨100⟩ direction of BCC lattice or axial direction of a defect, that the compressive stress increases the formation energy while the tensile stress results in an opposite trend [17–19]. MD results show that the interstitials in BCC iron can form a dislocation loop along the ⟨111⟩ direction when the number of interstitials is >4–5, even the initial state of SIAs in simulations was set as a parallel ⟨110⟩ cluster [6]. Thus, it is reasonable to consider, based on these state changes, that the coupling effect of temperature and stress would also induce a SIA-loop to migrate on free energy surface between different states. In this paper we will address such coupling effect on the states of nano-scale SIA dislocation loops by simulation and experimental methods to understand the properties of these nano-scale loops, which may be significant for further

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studying the radiation damage and developing radiation resistance materials.

The Ackland-2004 empirical Fe potential [20] is mainly employed in the present work. The initial 1/2 ⟨111⟩ dislocation loops are constructed by inserting three extra atomic layers on a {111} atomic plane along the ⟨111⟩ direction, in which its Burgers vector is perpendicular to the habit plane. The high elastic energy produced during the insertion is removed by moving the affected atomic layers related with the insertion according to the calculated displacement fields. The shape of the dislocation loop is determined as a hexagon or a circle according to the experimental observations [4–6,9]. The computation box consists of $34 \times 12 \times 21$ unit cells along X[111], Y[$11\bar{2}$]and Z[$\bar{1}10$] directions, respectively, consisting of 51,408 atoms in such matrix. The loops contain the number of interstitials from 19 to 151 in the computational boxes. Periodic boundary conditions are employed along the three directions during the simulations. The box with a loop is firstly relaxed with molecular static (MS) method. Then the MD simulations are performed with temperatures from 0 to 600 K in which the velocity scaling method is used. The uniaxial compressive or tensile stress along the Burgers vector (X direction) or perpendicular to the Burgers vector (along Y and Z directions) is applied at constant strain rates at each temperature with the same method described in Ref [21]. During the application of strain, the Poisson effect is considered along the directions perpendicular to the uniaxial strain direction, which is suitable for studying the uniaxial stress effect on samples. This method has been extensively and successfully used in the MD simulation of mechanical response in nanocrystal materials [20]. The time-step is chosen to be 1 fs. The experiments have also been performed with a 9%–12% Cr modified F/M steel (SIMP-steel) by 24 MeV iron irradiation during which the constant force is applied on sample at around 570 K. The initial stress is around 200 MPa. The experimental approach and results will be reported in detail elsewhere later. Here, we only discuss the related TEM studies to validate the simulation results.

The stress-strain (σ-ε) curve for the MD box containing a 1/2 ⟨111⟩ loop under the coupling condition is firstly calculated. Without stress, the temperature is found to only induce the change of the habit plane of a loop between {111}, {110} and {211} within MD time scale. Under applied stress at a given temperature, the σ-ε curve firstly shows a general feature of ductile material with the stress up to around 20 GPa, that is, the stress value increases continuously with the strain. Above 20 GPa, the σ-ε curve shows a turning point, which is defined as the ultimate stress point (USP), as shown in Fig. 1(a) (black line) for a system containing a 151-SIAs loop. It seems that the USP appears to be related with the configuration evolution of the dislocation loop, as explained in the following section. When the stress is smaller than the USP value for both compressive and tensile cases, the properties of the dislocation loop found to be remained as before, that is, the Burgers vector is still 1/2 ⟨111⟩ and the shape is also unchanged. However, in the region close the dislocation core, a large number of atoms moves to high energy states (potential energy, $E_{pot} > -3.85$ eV) under tensile stress, but an opposite trend is observed under compressive stress. These results may be explained by the higher/lower formation energy of a SIA under compressive/tensile stress respectively [17–19].

When the simulations are performed under the coupling condition with temperatures from 150 to 600 K and stress applied along the Burgers vector, the σ-ε curve also shows the USP as indicated in Fig. 1(a). The similar results are observed with the different loop sizes and strain rates. Under the tensile stress, the USP appears with the ε values around 0.148, 0.125, 0.108 and 0.099 at 150, 300, 450 and 600 K, respectively. Under the compressive stress, the temperature has less influence on the USP with the ε values ranged from −0.091 to −0.054. Comparing with the results obtained at 0 K, these results indicate that the coupling effect can readily lead to the state change of the system and induce the system to degenerate. The change of the habit plane is observed between {111}, {211} and {110} under the coupling effect. After the USP, the stress value decreases rapidly as shown in Fig. 1(a). However, neither micro-crack nor necking occurred just before and after the USP for all the cases studied here. Since the loop is the only special configuration in this system, the evolution of loop configuration is considered as a main reason to induce a discontinuity in the σ-ε curves.

In addition to the stress along the Burgers vector, the cases with the stress perpendicular to the Burgers vector are also studied, as shown in Fig. 1(b) (along Y direction). The result with the stress along Z direction is similar to the case along Y direction, which is not shown here. Fig. 1(b) exhibits that the stress increases with the strain before the USP and rapidly decreases after. The evolution of the loop configuration is also recognized as a main reason for the USP change. Comparing the σ-ε curves with the stresses along X and Y directions, it is clear that the USP can be easier established with the stress perpendicular than parallel to the Burgers vector under the tensile stress. In this case, the strain value at the USP is in the range from around 0.082 to 0.106 with decreasing temperature. Under the compressive stress, the results are contrary: the stress at the USP has a larger value with the stress perpendicular than parallel to the Burgers vector. The strain value at the USP is widely ranged from around −0.109 to −0.081. Hence, the tensile stress perpendicular to the Burgers vector can more easily change the loop configurations under the coupling effect.

The structural evolution of a loop under the coupling effect is then illustrated as following. Under the tensile stress, the configuration of a loop before the USP remains its initial shape and Burgers vector. After the USP, the loop decomposes into several small loops, as shown in Fig. 2(a). The central large loop remains the Burgers vector of 1/2[111], but degenerates into an ellipsoid shape, which is different from the 2D planar loop or other 3D SIA-cluster (C15 Laves phase) [22]. Six small loops are symmetrically around the central one with different Burgers vectors: 1/2[$\bar{1}$11], 1/2[1$\bar{1}$1] and 1/2[111]. Because the sum of Burgers vectors of these small loops are not equal to the Burgers vector of the original large dislocation loop, the Burgers vector conservation law is not satisfied. This is also confirmed by the TEM observations, as shown in Figs. 2(e) and (f), where the emission of small loops

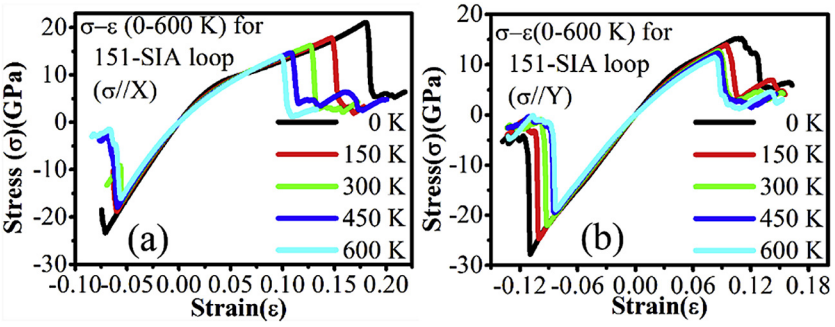

Fig. 1. Stress-strain curve for a system containing 151-SIA loop at different temperatures with the stress along (a) X [111] direction and (b) Y[$11\bar{2}$] direction.