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A molecular dynamics simulation study of irradiation induced defects in gold nanowire

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ABSTRACT

Displacement cascade in gold nanowires was studied using molecular dynamics computer simulations. Primary knock-on atoms (PKAs) with different kinetic energies were initiated either at the surface or at the center of the nanowires. We found three kinds of defects that were induced by the cascade, including point defects, stacking faults and crater at the surface. The starting points of PKAs influence the number of residual point defects, and this consequently affect the boundary of anti-radiation window which was proposed by calculation of diffusion of point defects to the free surface of nanowires. Formation of stacking faults that expanded the whole cross-section of gold nanowires was observed when the PKA's kinetic energy was higher than 5 keV. Increasing the PKA's kinetic energy up to more than 10 keV may lead to the formation of crater at the surface of nanowires due to microexplosion of hot atoms. At this energy, PKAs started from the center of nanowires can also result in the creation of crater because length of cascade region is comparable to diameter of nanowires. Both the two factors, namely initial positions of PKAs as well as the craters induced by higher energy irradiation, would influence the ability of radiation resistance of metal nanowires.

1. Introduction

Irradiation of metals with high energy particles results in displacement of atoms from their lattice sites. This leads to the production of various kinds of radiation damage, including point defects [1–3], defect clusters [4–6], dislocation loops [7] and stacking-fault tetrahedra (SFT) [8], in the material. These defects usually degrade the mechanical properties and thermal stability of the material. Besides the effects caused by collision cascade in the interior of material, the surface of materials also plays an important role in the result of radiation damage. Previous works which studied the effects of cascade occurred at the metal surface indicate that, in case of most energy of the incident ion is deposited in the vicinity of the surface, the pronounced damage caused by viscous flow or by microexplosion can lead to creation of large number of adatoms and vacancy dislocation loops beneath the surface [9,10], or even formation of craters on the surface [11–14].

Nowadays, materials with high radiation tolerance are very crucial for their applications in fission and future fusion reactors. The exploration of ion irradiation in nanolayered composites [15–18], nanocrystalline materials [19,20] and nanotwinned metals [21] shows that interfaces [22,23] and grain boundaries [24] can attract, absorb and annihilate the radiation induced defects, which leads to higher resistance to radiation of these materials as compared to the conventional bulk materials. Due to their importance and the promising applications of nanostructured materials in basic and applied research, the behavior of these materials under irradiation conditions have received a lot of multi-scale modelling investigations [25–29].

Since free surfaces are an unsaturated sink for absorbing point defects, the materials with large surface-to-volume ratio may exhibit high tolerance to radiation damage. Recently, nanoporous Au materials were proposed to have the ability of self-healing of the ion irradiation induced defects in a certain window which is defined by the size of the nanowire and the dose rate of ions [30]. Due to the fact that nanowires are promising candidates for stronger radiation tolerance than traditional bulk materials, therefore the response of nanowires under ion-bombardment have been extensively studied in recent years. The study which utilized high resolution transmission electron microscope (TEM) along with

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molecular dynamics (MD) simulation found that SFT is formed in Au nanowire at high dose-rate but is absent at low dose-rate. That work confirms radiation tolerance of nanowire below certain dose rate [31]. The *in situ* TEM observations of Kr ion irradiation of silver nanowires found that the surface can absorb various kinds of defects including individual dislocation loops and SFTs [32]. That is a direct experimental observation of self-healing of the irradiation induced defects. A competition between the attractive force among the vacancies in cascade region and absorption of point defects by the free surface, that influences the window of radiation endurance of the gold nanowires, was also proposed [33]. The study of single-ion impacts on the surface of gold nanorods observed an enhanced sputtering yield and MD simulations explained that the reason for this is explosive ejection of nanoclusters [34]. The influence on mechanical properties of the nanowires under irradiation was also studied by several MD simulation works [35–38].

In this article, different irradiation conditions, namely with various PKAs' kinetic energies and initial positions, were employed in MD simulations. The purpose of this work is to obtain the response of nanowires bombarded with increasing PKAs' energies, as well as to study the influence of diameter and surface of nanowires on the production of radiation damage. We found that initial positions of PKAs have impact on the residual number of point defects. And the reason has been analyzed in this work. With increasing PKAs' kinetic energy, the stacking faults and crater at surface can be formed in gold nanowire. The mechanisms of formation of these two kinds of defects were fully discussed in this work. To the best of our knowledge, this is the first detailed study that proposed the formation of cascade induced crater will degrade the window of radiation endurance of gold nanowires.

2. Methods

Simulation package LAMMPS [39] was used to carry out the MD simulation of displacement cascade in gold nanowires in this work. At the beginning, a single crystalline gold nanowire was constructed. In the nanowire, ⟨100⟩ and ⟨010⟩ directions are along the radial direction, and ⟨001⟩ direction is along the axial direction. The periodic boundary condition (PBC) was applied only along the axial direction, the other two directions were free surfaces. The nanowires with different diameters of 5.7 nm, 8.2 nm, 10.6 nm and 13.8 nm were implemented in this work. The ratio of length-to-radius was kept as 4 for all nanowires to guarantee the cascade can propagate freely along the axial direction and it was not influenced by the PBC applied.

The embedded atom method (EAM) potential for Au [40] was used to describe the interactions of Au atoms around the equilibrium distance. In order to correctly model the cascade process in which the atoms may reach a distance very close to each other, the EAM potential was smoothly splined to universal screened Ziegler-Biersack-Littmar (ZBL) potential [41] within a short distance. In our work, we followed the joining method used by Zhang et al. [33] earlier. In their article, a third order exponential polynomial was used to join the effective charge of EAM and ZBL potentials, which is shown by Eq. (1). The detailed procedure about the joining method can be found in Ref. [33].

$$Z(r_{ij}) = \begin{cases} Z_{ZBL}, & \text{if } r_{ij} \leqslant r_1; \\ exp(b_0 + b_1 r_{ij} + b_2 r_{ij}^2 + b_3 r_{ij}^3), & \text{if } r_1 \leqslant r_{ij} \leqslant r_2; \\ Z_{EAM}, & \text{if } r_{ij} \geqslant r_2. \end{cases} \quad (1)$$

In our work, the joining points, r_1 and r_2, are slightly different from those in Ref. [33]. And the whole set of parameters that we used is shown in Table 1.

After the initialization, the nanowires were firstly relaxed using the conjugate gradient method and then equilibrated at 300 K with NPT ensemble for 100 ps with a time step of 1 fs, so as to reach the equilibrium state at the given temperature. After the relaxation, PKAs with different kinetic energies were created either at the surface or at the center of the nanowires. PKAs with kinetic energy of 1 keV were introduced to investigate the effect of different PKAs' positions on the generation of point defects. Nanowires with diameters of 8.2 nm and 13.8 nm, under self-bombardment with PKA energies of 5 keV, 10 keV, 15 keV and 20 keV, were also simulated to find out the response of nanowires irradiated under higher PKA energies. In all these simulations, the direction of PKA's velocity was kept along the ⟨010⟩ direction which is normal to the surface of nanowires.

After a PKA was induced, the NVE ensemble was applied to the system. In order to simulate the energy dissipation to the surrounding atoms at the ends of the nanowire, the velocity rescaling method was applied to the atoms with thickness of two atomic layers at the both ends. During the cascade simulation, variable time steps were applied in order to ensure that the maximum distance one atom can travel during the cascade process was no more than 0.02 angstrom. All of the cascades were evolved for 80 ps, which can guarantee that there is no rapid structure changes happened anymore and a stable defect configuration was established within the MD simulation time. In order to reduce the statistical error, 30 independent cascade simulations were conducted at each identical irradiation condition (same PKA energy, position and same nanowire size) in case of PKA's energy is equal to 1 keV. In addition, 10 independent simulations were carried out if PKA's energy is higher than 5 keV. In the circumstances of higher energy irradiation under which stacking faults may form, further annealing at 300 K with NPT ensemble was applied to observe the structure evolution of the stacking faults. For comparing the number of point defects in nanowires with its number in bulk Au, cascade simulations with PKA energies of 1 keV were also performed at the center of a single Au crystal.

Visualization of the results of simulations was realized by using OVITO [42]. Surface region of the nanowire is defined as the outmost one atomic layer, which is along the radial direction with thickness of about 0.4 nm. And the remaining part is defined as the interior region of the nanowire. Atoms moved away from the surface with a distance larger than 2.4 nm are considered as sputtered atoms. We used Wigner–Seitz analysis method to identify the self-interstitial atoms (SIAs) and vacancies of the damaged nanowires. The thermally equilibrated nanowires were taken as the reference configuration in Wigner–Seitz method. The common neighbor analysis (CNA) [43] is used to distinguish the arrangement of atoms into different categories, including those in face-centered-cubic (FCC), hexagonal-close-packed (HCP), body-centered cubic (BCC) and the others. Fig. 1 gives the configuration of a gold nanowire with diameter of 8.2 nm after the equilibration at 300 K with NPT ensemble. The surface atoms and crystallographic orientations are also displayed in different colors.

3. Results and discussion

3.1. Point defects

Since the surface of nanowires is a perfect sink for the defects induced by irradiation, many point defects and defects clusters will migrate to the surface during or after the cascade. Nevertheless, the number and distribution of point defects left inside the nanowire is very crucial for their subsequent migration beyond the MD simulation time, as well as it is the key factor that influences the mechanical property of the nanowire [36,38]. Due