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A molecular dynamics study of helium bombardments on tungsten nanoparticles

Min Li*, Qing Hou, Jiechao Cui, Jun Wang

Key Laboratory of Radiation Physics and Technology, Ministry of Education, Institute of Nuclear Science and Technology, Sichuan University, Chengdu 610064, PR China

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ABSTRACT

Molecular dynamics simulations were conducted to study the bombardment process of a single helium atom on a tungsten nanoparticle. Helium atoms ranging from 50 eV to 50 keV were injected into tungsten nanoparticles with a diameter in the range of 2–12 nm. The retention and reflection of projectiles and sputtering of nanoparticles were calculated at various times. The results were found to be relative to the nanoparticle size and projectile energy. The projectile energy of 100 eV contributes to the largest retention of helium atoms in tungsten nanoparticles. The most obvious difference in reflection exists in the range of 3–10 keV. Around 66% of sputtering atoms is in forward direction for projectiles with incident energy higher than 10 keV. Moreover, the axial direction of the nanoparticles was demonstrated to influence the bombardment to some degree.

1. Introduction

Currently, because of unique physical and chemical properties, nanoparticles are applied in various industries [1–3], and the corresponding ion irradiation of nanoparticles has been investigated widely in experiments. In some cases, the response of nanoparticles to ion irradiation differs greatly from that of bulk materials. Thus, many experiments have been designed to modify the nanoparticles and to measure the sputter yield [4,5]. Recently, another category of experiments has emerged – the irradiation of dust particles in space or in a plasma environment.

Tungsten (W) has been selected as the plasma-facing material (PFM) [6] in nuclear fusion reactors due to its excellent physical properties and stable chemical properties. W dusts have also been confirmed to be produced in fusion devices [7]. These dusts on a nanometer scale can be forced to move easily in the chamber or to impact PFM. During their movement, there is a probability of them colliding with helium (He) atoms. The results of such a collision are unclear. Thus, it is necessary to study the bombardment of an He atom on W nanodust. The detail of the underlying atomic process is difficult to investigate directly in experiments, which is also of scientific interest. In addition, nanoparticles in most experiments are supported on a surface and thus produce different results than experiments with free nanoparticles would. Therefore, theoretical studies are needed. Molecular dynamics (MD) simulation is one of the most powerful methods for the investigation of nanoparticles.

A considerable number of MD simulations have concentrated on heavy atom bombardments. For example, MD simulations have been applied to study energetic gold (Au) atom bombardment on Au clusters with radii up to 10 nm [8–10]. Järvi et al. [11,12] carried out MD simulation to study the sputtering of Au nanoparticles with radii up to 8 nm using 25 keV gallium (Ga) ions. The sputtering was found to be maximized as a function of sphere radius when the ion penetration depth is of the order of the sphere radius. In a recent work, using MD simulation, Sandoval et al. studied the sputtering of Au nanoparticles by 200 keV xenon (Xe) impact and proved that the sputter yield of supported nanoparticles is estimated to be around 80% of that of free nanoparticles due to the suppression of forward sputtering [13].

Seldom have MD simulations included He atom bombardment on W clusters. The bombardment result for both projectiles and nanoparticles will differ from that of heavy projectiles. Previously, we have successfully investigated He bombardments on W surfaces, the melting and dissociation of free nanoparticles, and the coalescence between nanoparticles with MD simulations [14–17]. In this study, we focused on the interaction between He atoms and W nanoparticles with diameters ranging from 2 to 12 nm.

2. Method

To improve computational efficiency, a Molecular Dynamics Package of Sichuan University (MDPSCU) with graphics processing units (GPUs) for parallel computing was used [18]. A Finnis-Sinclair-type potential obtained by Ackland et al. [19] was adopted to describe the interaction between W atoms. For the He-W potential, the short

* Corresponding author.
E-mail address: limin126@scu.edu.cn (M. Li).

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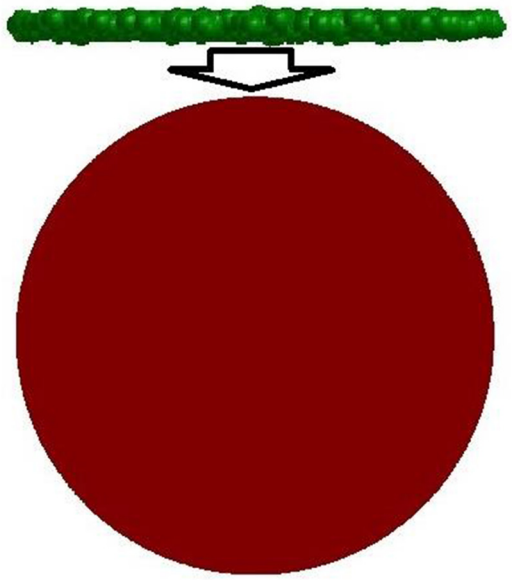

Fig. 1. Simulation model for bombardment of a single He atom on a W nanoparticle. 1000 simulation samples have been superimposed together. Green dots: 1000 He atoms; red dots: nanoparticle atoms. The arrow represents the incident z-direction of projectiles. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

range part was based on the Ziegler-Biersack-Littmark (ZBL) potential [20], while the long range part was constructed by fitting ab initio data, and the two parts were connected smoothly [21].

For the preparation of W nanoparticles, a cubic W box containing 128,000 atoms at 0 K was created first. Then, W nanoparticles with diameters in the range of 2–12 nm were cut from the box. For each size, 1000 nanoparticle samples were cut with their centers chosen randomly in the box and then rotated randomly. The temperature of each nanoparticle was increased gradually from 0 K to 1500 K by adopting an electron-phonon coupling model (EPC) proposed by Finnis et al.[22], which had been used for simulating the depositions of Au clusters on surfaces [23] and the bombardments of He atoms on W surfaces [14]. Next, a single He atom was given an initial energy in the range of 0.05–50 keV and struck one nanoparticle perpendicularly, as shown in Fig. 1. The projectile was placed 1.2 lattice length a_0 distance above each nanoparticle, where a_0 was set as 3.1652 Å. The *x*- and *y*-positions of the projectile were chosen randomly in a circle above the corresponding nanoparticle. The circle has the same diameter as the nanoparticle to be bombarded. In Fig. 1, as 1000 nanoparticle samples with different axial directions are illustrated together, the superimposed nanoparticles seem like a ball. To investigate the influence of axial direction on the interaction of projectiles and nanoparticles, another 1000 nanoparticles with their ⟨0 0 1⟩ directions parallel to the *z*-direction were bombarded. Each bombardment process lasted at least 10 ps. Subsequently, the changes to the projectiles and nanoparticles were studied.

To compare the differences in the bombardments of He atoms on nanoparticles and bulk, we prepared a $30\,a_0 \times 30\,a_0 \times 30\,a_0$ (0 0 1) cubic box at 1500 K as the bombarded substrate. For each unit of projectile energy, 1000 independent bombardments were carried out. The colliding atoms were also placed $1.2\,a_0$ distance above the substrate with the incident direction normal to the surface, and the *x*- and *y*-positions of the projectile were chosen randomly. The periodic conditions were applied in the *x*- and *y*-directions. Each simulated process lasted 15 ps. Special attention was paid to 100 eV He atom bombardment on (0 0 1) substrate in order to obtain depth distributions for comparison with in nanoparticles. For this special simulation, 7600 runs were performed.

3. Results and discussion

3.1. Reflection and deposition of He atoms

The total number of He atoms reflected from the 1000 nanoparticles at 1500 K at different times was calculated and defined as N_{refl}. The relationship between N_{refl} and projectile energy E_k was investigated. Take 4 nm-nanoparticle and 12 nm-nanoparticle as examples, the results of which are shown in Fig. 2. For all E_k values, N_{refl} evolves with the same tendency. First, after He atoms have arrived at the 1000 nanoparticles, they start to reflect slowly early on. That is because most projectiles are still moving forward in nanoparticles. For lower projectile energy, they need more time to arrive at nanoparticles; thus, the emergence of their reflection is delayed. Subsequently, He atoms are reflected out quickly due to their collision with nanoparticle atoms. The rapid reflection process lasts no more than 0.5 ps. After the period, the reflection is slowed down, especially for projectiles with E_k no more than 1 keV. Thermal diffusion of the He atom is the main reason leading to the escaping from nanoparticle in this stage, similar to the reflection of He atom from bulk W as we reported in Li et al. [14]. Comparing Fig. 2(a) and (b), the larger the nanoparticle is, the more He atoms it retains. Therefore, the thermal release is obvious for larger nanoparticles. For projectiles with E_k higher than 10 keV, most of them penetrate through nanoparticles and only a few are reflected. Finally, N_{refl} remains nearly stable.

The total number of He atoms trapped in the 1000 nanoparticles at 1500 K at various times was calculated and defined as N_{in}. The

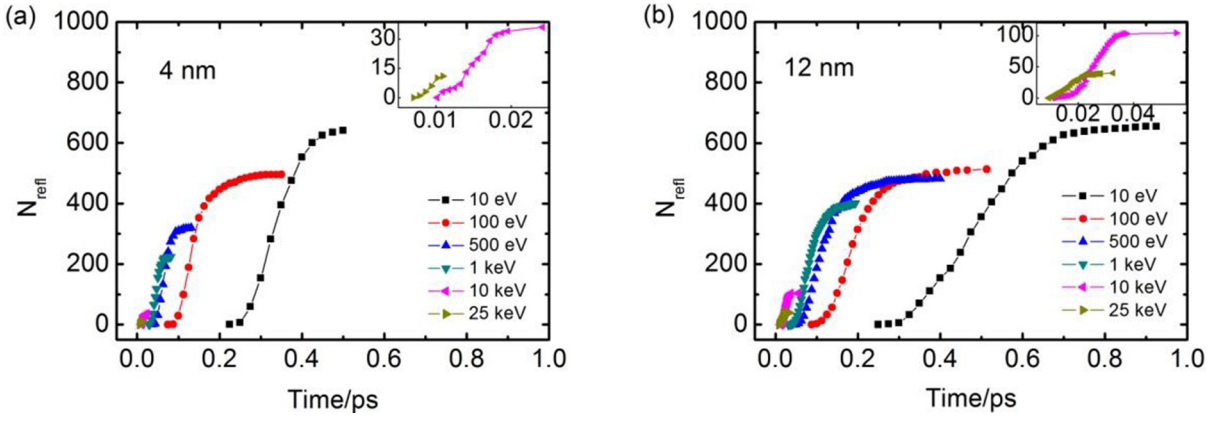

Fig. 2. The relationship between the total number of reflected He atoms N_{refl} and E_k for (a) 1000 4 nm-nanopartiles and (b) 1000 12 nm-nanopartiles at various times. The insets show the high-energy curves (10 keV and 25 keV) more clearly.