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Research Article

Influence of Irradiation on Mechanical Properties of Nickel

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The influence of irradiation on mechanical properties of nickel is studied using molecular dynamics (MD) simulation. The single crystal nickel is irradiated with the primary knocked-on atom (PKA) energies of 5 keV, 10 keV, 20 keV, and 30 keV at 300 K, and then the tensile test is performed. The simulation results reveal that the yield strain and yield stress of irradiated nickel decrease with the irradiation energy increasing, while the elastic modulus has no obvious change at various irradiation energies. By analyzing the stress-strain curves and the microstructure evolution, it is found that the effect of irradiation accelerates the damage of the internal structure due to the existence of irradiation defects, and high-energy irradiation leads to the instability of the structure in the process of plastic deformation.

1. Introduction

With the increasing demand for traditional fossil energy, the energy shortage has become one of the major issues of human existence. By contrast, the nuclear fusion energy is considered to be one of the important forms for solving the problems of energy and environment in future because of the abundant resources, huge reserves, and the characteristics of clean and safety. With the development of international thermonuclear fusion reactors, it is able to offer the important way for obtaining the controlled nuclear fusion energy. In the fusion reactor, the first wall materials are often under the action of sputtering, foaming, and corrosion of plasma escaping particles. These irradiation effects cause changes in the microstructure, such as formation of vacancies, voids, dislocation loops, and stacking fault [1–4], which will lead to irradiation hardening, irradiation embrittlement, and the decrease in mechanical properties so that the stability and security of the material are seriously affected [5–7]. Thus, the irradiation effect has an important influence on the mechanical properties of materials.

In recent years, the research on mechanical properties of metallic materials has been a hot topic at home and abroad. As the research on the irradiation mechanical properties of metallic materials is mainly by tests, there is little research on theory. The results show that the interaction of the dislocation movement and irradiation defects causes the decreasing of the materials' mechanical properties during the tensile process when the metal materials are irradiated [5, 8–10]. For instance, Li simulated the mechanical properties of irradiated copper using molecular dynamics simulation and showed that the compressive Young's modulus of copper increased, while the tensile Young's modulus decreased after irradiation [11]. Carpenter et al. studied the mechanical properties of irradiated single-layer graphene and found that the vacancy-induced crystalline to amorphous transition was accompanied by a brittle-to-ductile transition in the failure response of irradiated graphene sheets, and the point defects and large voids appreciably degraded the strength of pristine graphene [12]. At present, as the research on nickel mainly focuses on the field of irradiation damage, the results present that various types of defects, such as vacancies, voids, stacking-fault tetrahedra, and interstitial dislocation loops, are formed in the internal structure of the crystal [13–15]. However, the study on mechanical properties of irradiated nickel is still not conducted.

So this study effectively analyzes and predicts the mechanical properties under the condition of irradiation for guiding the design of plasma-facing materials.

This paper is focused on investigating the mechanical properties of irradiated nickel at various energies of primary knocked-on atoms. In the process of research, the molecular dynamics (MD) simulation is used in the tensile test, and the software of Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is used to study the influence of irradiation on mechanical properties of nickel [16]. The microstructure evolution is analyzed with common neighbor analysis (CNA) proposed by Honeycutt and Andersen [17], which provides the details of evolution process of the microstructure. The change in yield stress, yield strain, and elastic modulus is discussed after irradiation for single crystal nickel.

2. Atomistic Model and Simulation Method

Figure 1(a) shows the initial model of single crystal nickel. The x, y, and z directions are [100], [010], and [001], respectively, and the dimensions of the box are $60a \times 60a \times 60a$, where a is the lattice constant (0.35157 nm). The model contains 864000 atoms, and the periodic boundary condition is applied in the x, y, and z directions. We choose an atom as the primary knock-on atom (PKA) from the initial model of single crystal nickel as shown in Figure 1(b). Then, the energies of 5 keV, 10 keV, 20 keV, and 30 keV are applied to the PKA, and the cascade collision is along [135] direction. In the process of molecular dynamics simulation, applying 16 cups for parallel computation, the models are equilibrated under NPT ensemble at 300k, a Nosé–Hoover thermostat is applied to maintain the system temperature, and the simulation time is 20 ps. Then, the NVE ensemble is used to simulate the process of cascade collision, and the time steps range from 0.01 fs to 1 ps and the test is performed for 60 ps. When the cascade collision stopped, the samples are fully relaxed to equilibrium. And then we calculate the number of defects after cascade collision with the increase in PKA energies, as shown in Figure 2, and the results present that the defect numbers increase with the PKA energies increasing. Finally, the uniaxial tensile test is performed for all the irradiated samples in the z direction using molecular dynamics simulation with the time integration step of 1 fs under NPT ensemble, and the simulation time is about 300 ps.

In the molecular dynamics simulation, the interactions between atoms are described by a modified analytic embedded atom method (MAEAM), which has been applied successfully in the studies of metallic microstructures and melting simulations [13, 18–21]. The MAEAM is a type of EAM potential and its formalism is

$$E_i = \frac{1}{2}\sum_{j\neq i}\varphi\left(r_{ij}\right) + F\left(\rho_i\right) + M\left(P_i\right), \qquad (1)$$

where $\varphi(r_{ij})$ is the pairwise interaction, $F(\rho_i)$ present the embedding energy, and $M(P_i)$ is an extra energy-modified term that represents the contribution of nonspherical symmetry coming from each neighbor atom j with respect to the spherically symmetric atomic electron density.

3. Mechanical Properties of Irradiated Nickel

3.1. Analysis of Stress-Strain Curves. Figure 3 shows the variation in stress-strain curves of the irradiated and unirradiated nickel during the tensile test at room temperature. The results present that the maximum stress of unirradiated nickel is up to 14.9 GPa when the strain is 11.8% and the PKA energy is 5 keV, but nickel, after irradiation, has a maximum stress of 13.36 GPa and strain of 10.07%. So, it can be concluded from the stress-strain curves that the mechanical properties of nickel decreased with the increase in irradiation energy. In order to obtain the influence rules of irradiation on mechanical properties, the values of the yield strain, yield stress, and elastic modulus of nickel are extracted from the stress-strain curves, as shown in Table 1. The results show that the yield stress and yield strain consistently decreased when irradiation energies increased. Meanwhile, the elastic modulus of single crystal nickel before and after irradiation is also calculated according to the rule $E = \sigma/\varepsilon$, and the results show that the elastic modulus of unirradiated nickel is 127 GPa, and after irradiation, it increases from 127 GPa to 132 GPa with the raise in irradiation energies. But when the irradiation energy is up to 30 keV, the elastic modulus of nickel declines compared with unirradiated nickel. It indicates that high-energy irradiation severely destroys the internal structure of the crystal, resulting in hardening and instability of the structure.

Besides, some information about plastic deformation from the curves of stress-strain can be obtained. The curve of plastic deformation region is smooth and slow for unirradiated nickel, and when the energies of PKA are 5 keV and 10 keV, it has the similar fluctuation. But as the energies of PKA are up to 20 keV and 30 keV, the curves of plastic deformation region present a wide range of fluctuation. Thus, it can be concluded that the plastic deformation is stabile in low irradiation energies, which is similar to the range before irradiation, but high energies induce the instability of plastic deformation.

3.2. Evolution of Microstructure before and after Irradiation. Figure 4 shows the microstructure evolution of the plastic deformation region of unirradiated nickel during the tensile test at room temperature. It is clear that the main deformation mechanisms are slip bands, and there are some cross slip bands (denoted in red atoms) with increasing strain, as shown in Figure 4; the slip systems are {111}<110>. Many slip interfaces (presented by white atoms in Figure 4) appear at the end of the slip bands. But the deformation characteristics change after irradiation of nickel. Figure 5 presents the microstructure evolution of irradiated nickel during the tensile test at room temperature when the energies of PKA are 5 keV and 10 keV. Compared with the unirradiated nickel, the deformation mechanism of irradiated nickel remains the slip bands, but the number of slip bands significantly decreases after irradiation. In Figure 5(a), when the irradiation energy is 5 keV, the inside of the crystal generates many irradiation defects, which inhibit the extension of slip in the process of plastic deformation so that

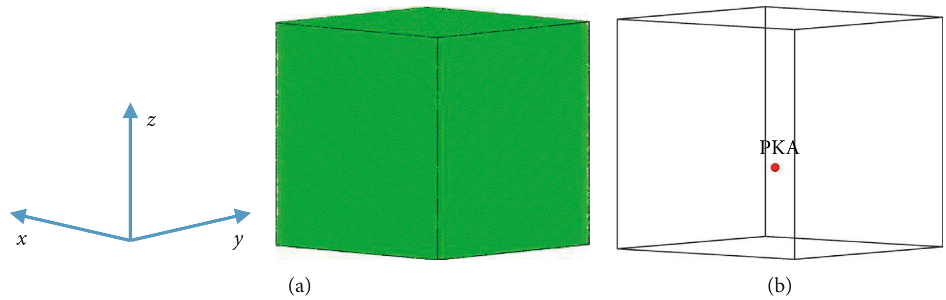

Figure 1: The initial model of single crystal nickel.

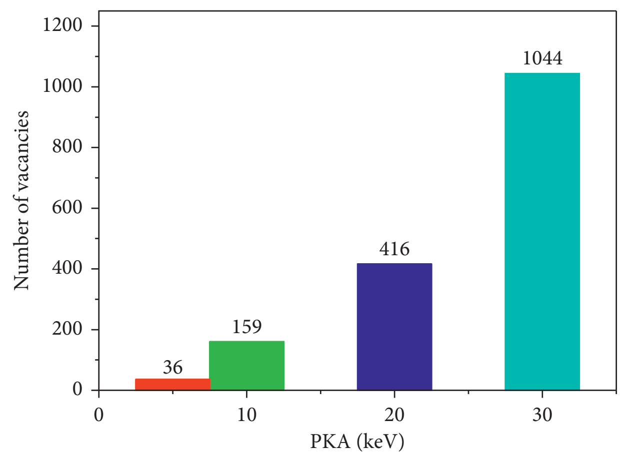

Figure 2: Variation in defect numbers with the increasing energies of PKA.

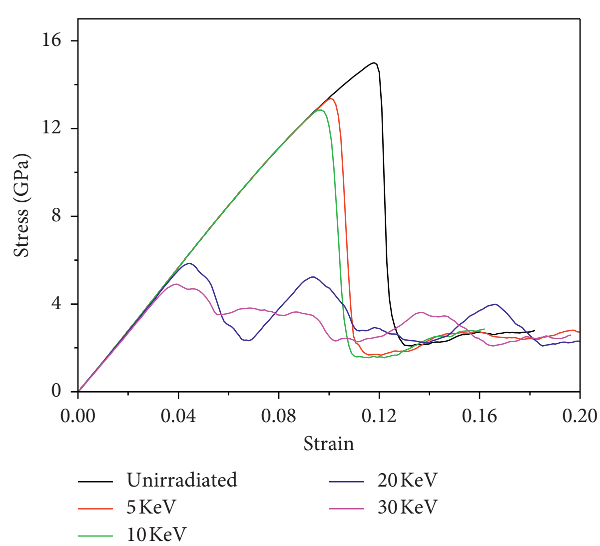

Figure 3: Stress-strain curves for irradiated Ni during the tensile test at room temperature.

the density of slip bands decrease. At the same time, the irradiation defects appear due to the stress concentration. In order to relax the stress concentration, multilayer slips are formed, which become the main deformation characteristic, so the plastic zone of the irradiated nickel is larger than that of the unirradiated nickel. In Figure 5(b), when the irradiation energy is up to 10 keV, the effects of multilayer slips are more evident, and the number of slip bands increases compared with the situation of 5 keV. The main reason is that the irradiation defects increase with the increase in the

Table 1: Calculated values of the yield strain ($\varepsilon_{\text{yield}}$), yield stress ($\sigma_{\text{yield}}$), and elastic modulus ($E$) for single crystal Ni at room temperature.

Ni	$\varepsilon_{\text{yield}}$ (GPa) (%)	σ_{yield} (GPa)	E (GPa)
Unirradiated	11.8	14.997	127.09
5 keV	10.07	13.369	132.76
10 keV	9.7	12.837	132.36
20 keV	4.51	5.848	129.66
30 keV	3.94	4.909	124.59

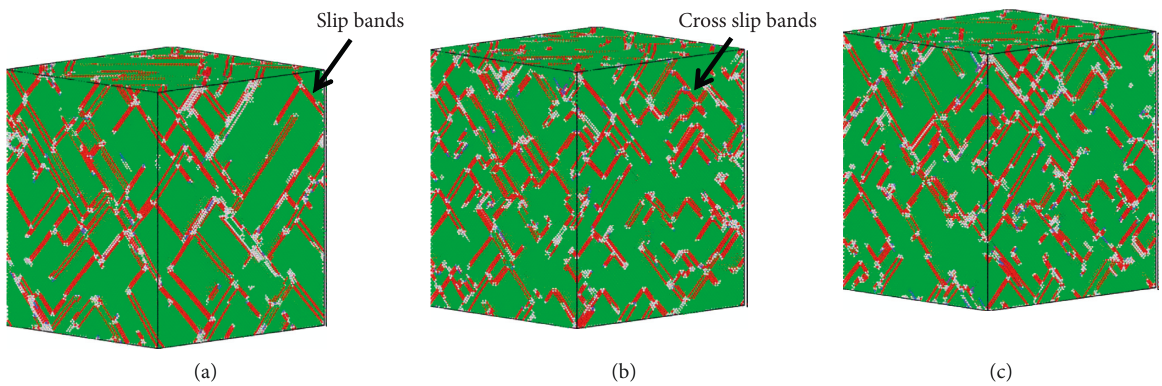

Figure 4: Microstructure characteristics for the unirradiated Ni during the tensile test at room temperature: (a) 12%, (b) 12.2%, and (c) 12.3%.

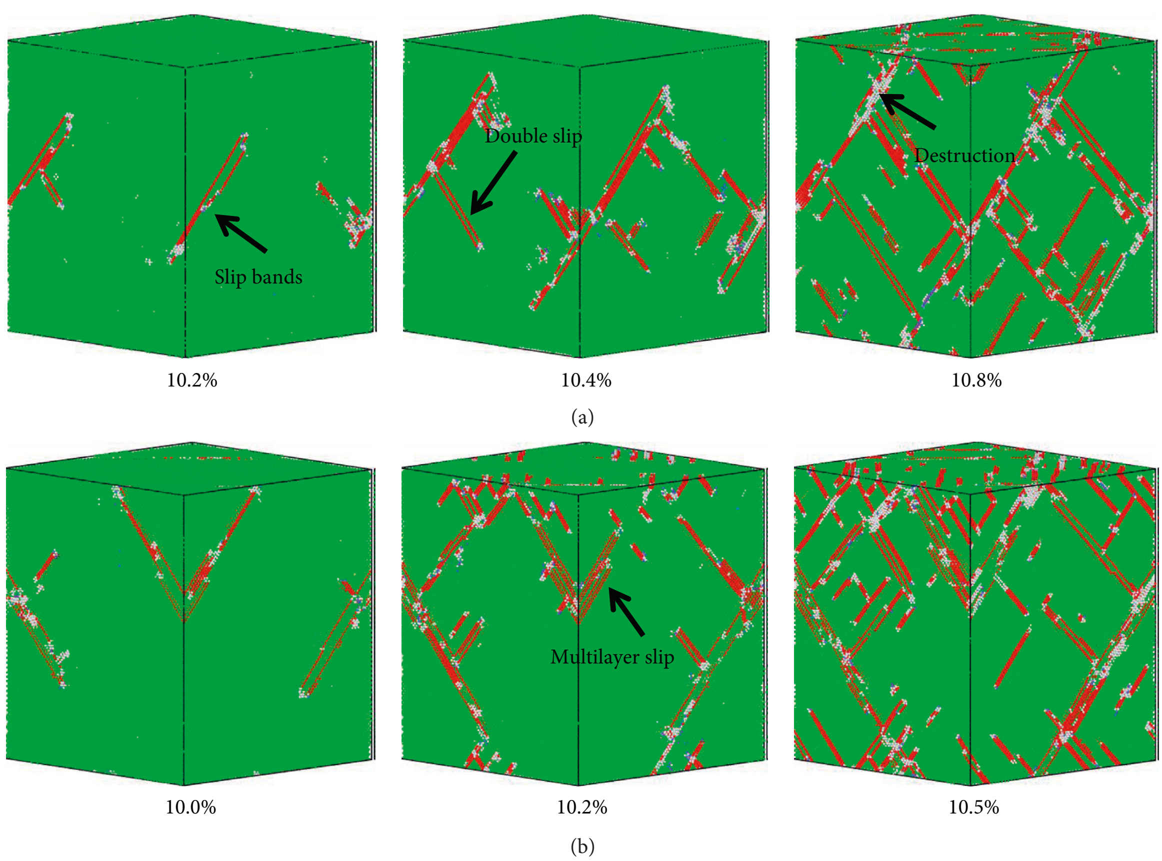

Figure 5: Microstructure evolution for irradiated Ni during the tensile test at (a) 5 keV and (b) 10 keV.

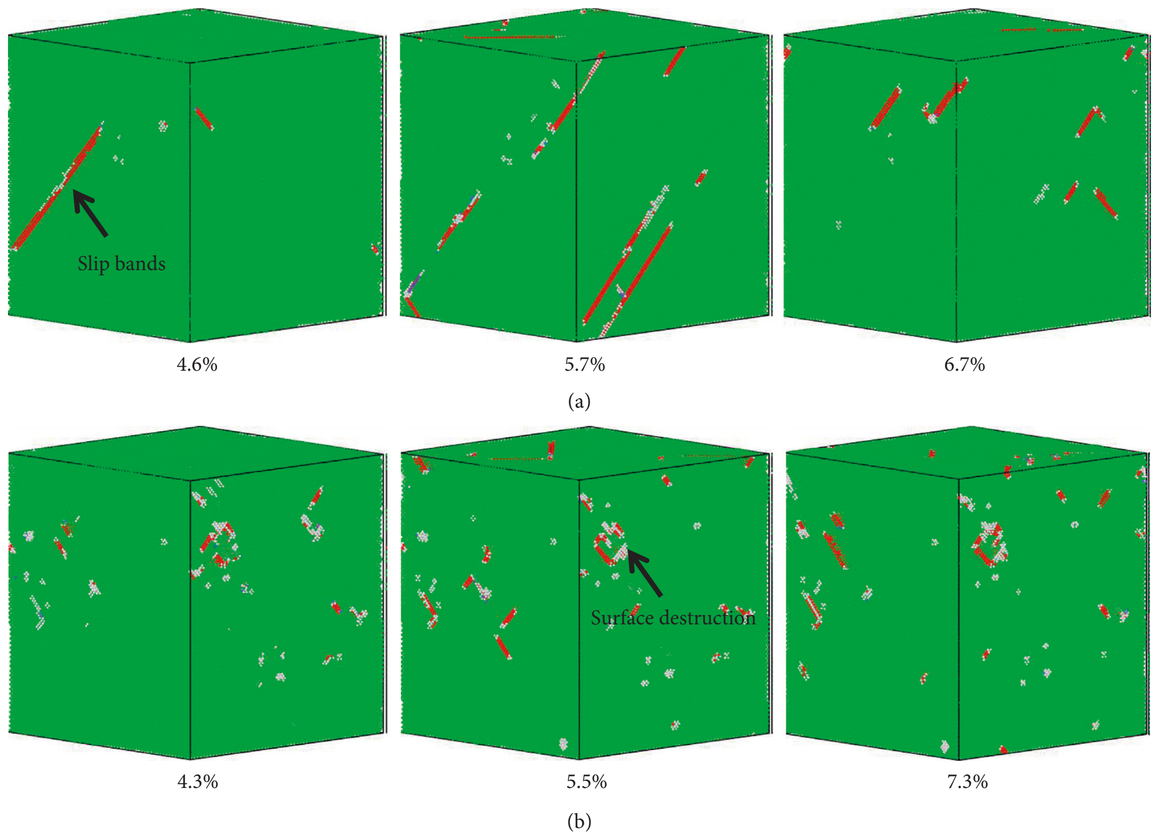

FIGURE 6: Microstructure characteristics for irradiated Ni during the tensile test at (a) 20 keV and (b) 30 keV.

irradiation energy, as shown in Figure 2, so more plastic deformation is needed to relieve the stress concentration around the irradiation defects, and much interface failure occurs at the end of slip bands.

As the irradiation energies are increased to 20 keV and 30 keV for nickel, the plastic deformation characteristics change in the uniaxial tensile test, as shown in Figure 6. The obvious change is that the plastic deformation reduces and the surface failure increases as a result of the influence of low energy irradiation from structure evolution, as shown in Figure 6(a), and the slip bands almost disappear at a high irradiation energy of 30 keV, as shown in Figure 6(b), where there is only a small amount of short slips are formed and the surface structure is seriously destroyed. One of the major reasons is the formation of high stress zone around the defects during the tensile test; hence, the interior structure is destroyed.

4. Conclusion

The influence of irradiation damage on mechanical properties of nickel is studied using molecular dynamics simulation. The single crystal nickel is irradiated with the energies of primary knocked-on atom (PKA) of 5 keV, 10 keV, 20 keV, and 30 keV at 300 K, and then the tension test is performed. The simulation results reveal that the yield strain and yield stress of irradiated nickel decrease with the increase in irradiation energy, while the elastic modulus has no obvious change at various irradiation energies. By analyzing the stress-strain curves and the microstructure deformation, it is found that the effect of irradiation accelerates the damage of the internal structure, reducing the number of slip bands, and high-energy irradiation leads the slip bands to disappear and decreases the instability of the structure in the process of plastic deformation.

Data Availability

The calculated data used to support the findings of this study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

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