Research Article

Effect of Nanoindentation Temperature on Plastic Deformation of 3C-SiC Based on the Molecular Dynamics Method

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To explore the effect of nanoindentation temperature on the plastic deformation of 3C-SiC, it is possible to analyze the 3C-SiC load-displacement changes at different temperatures and the dislocation propagation in the plastic deformation stage. The 3C-SiC nanoindentation model is established on the basis of molecular dynamics interatomic interaction potential. The model combines the 3C-SiC crystal structure to optimize the Vashishta potential function and modifies the relaxation system, system boundary, and other simulated environmental factors. The plastic deformation process of 3C-SiC at different temperatures is analyzed from multiple angles such as the load-displacement curve, the stress distribution during the plastic deformation stage of the matrix, and the formation and growth of specimen dislocations. During the pressing process, intermolecular dislocations and stress are concentrated in the elastic-plastic deformation zone. The load value of the elastic-plastic deformation zone under high temperature environment is generally higher, and the energy of the dislocation loop will be released. In the plastic deformation zone, the dislocation loop will break under the action of high temperature environmental load. The premature release of energy will cause the load value to drop. During the pressing process, the bearing capacity of 3C-SiC polycrystalline will decrease as the temperature rises. Plastic deformation occurs inside the material, and dislocations nucleate and expand from the grain boundary to the crystal and finally form a U-shaped dislocation ring.

1. Introduction

Silicon carbide ceramic bearings have the advantages of lightweight, high hardness, and high temperature resistance [1–3]. It has been widely used in the fields of aerospace, defense and military, metallurgical industry, and other fields [4, 5]. Silicon carbide ceramic bearings have excellent mechanical properties, and these excellent macroproperties are essentially determined by their microstructure [6]. However, the mechanism by which the microstructure affects the macroscopic mechanical properties is still unclear, and the cross-scale research from the microstructure to the macroscopic properties has become a current hot and difficult point [7–9]. The molecular dynamics method can dynamically simulate and observe the changes in the state of each atom in the system [10]. Observing the evolution of the fine structure inside the material has become an effective calculation method in the auxiliary research of microcontact science and experimental methods [11–13].

Many researchers explore the influencing factors of material deformation mechanism based on molecular dynamics simulation [14–16]. Yuanji et al. [17] studied the plastic deformation mechanism of polycrystalline α-silicon carbide matrix under the action of nanoindentation under the conditions of considering the effects of grain boundaries and temperature. The study found that as the temperature increases, the load-bearing capacity of the α-silicon carbide polycrystal decreases, and plastic deformation occurs inside the material. Zhang et al. [18] used a molecular dynamics approach to initially investigate the Hugoniot properties of α-silicon carbide. The impact-induced plastic deformation in α-silicon carbide was found to exist mainly in the form of deformation twins. Tian et al. [19] used molecular dynamics simulations to perform scribing experiments on...
the 6H-SiC surface to study the material removal of its subsurface defects. It was found that the deformation of the material mainly consists of plasticity, amorphous transition, and dislocation slip, the C phase has less amorphous deformation compared to Si, and the material removal is better. The abovementioned literature has mainly studied single-crystal and polycrystalline materials, and the microstructure of 3C-SiC materials at different temperatures and their deformation mechanisms is not clear.

In this paper, considering the temperature effect, the Vashishta potential function is established based on the molecular dynamics method. Mainly study the deformation mechanism of 3C-SiC specimens under the action of nanoindentation at 10K, 300K, 600K, and 900K temperatures. Among them, the load-displacement curve of 3C-SiC specimens at different temperatures, the stress distribution at the stage of matrix plastic deformation and the formation and growth of specimen dislocations are analyzed. By exploring the internal dislocation phase and stress distribution of 3C-SiC, we can deeply understand its elastoplastic transformation mechanism. Describe the atomic destruction and migration trajectory changes in the deformed area by identifying the deformed structure and analyze the load-displacement curve. Explore the influence of different ambient temperatures on the elastoplastic deformation of 3C-SiC under nanoindentation.

2. The MD Simulation Model of 3C-SiC Nanoindentation

2.1. The Establishment of the Nanoindentation Model. The schematic diagram of 3C-SiC three-dimensional indentation simulation is shown in Figure 1. The 3C-SiC indentation specimen is a rectangular parallelepiped, and the dimensions in the X, Y, and Z directions are 24.00 nm × 24.00 nm × 17.00 nm, respectively. The cuboid specimen contains 1021520 atoms, including 510760 C atoms and 510760 Si atoms. The diamond indenter is composed of C atoms, and because of its extremely high hardness, it is regarded as a steel body. The shape of the indenter is a combination of a cylinder and a cone. The diameter of the bottom circle of the cylinder is 8.00 nm, and the height is 6.23 nm, The cone height is 3.26 nm and contains 115845 C atoms in total. The initial distance between the top of the indenter is 0.20 nm from the test piece, and the indenter moves downward to press into the sample during the indentation process. All molecular dynamics indentation simulations are performed with a constant time step of 1 fs. The conjugate gradient (CG) algorithm is used to optimize the sample before the indentation simulation, so that the system reaches the minimum equilibrium energy and is in a stable state. In order to prevent the substrate from moving during the indentation process, the atoms at the bottom of the sample are fixed. The boundary conditions in the Z direction are set as fixed boundary conditions, and the boundary conditions in the X and Y directions are, respectively, set as periodic boundary conditions.

2.2. Interatomic Potential. The potential function describes the interaction potential between atoms in the system and is the core factor that determines the accuracy and reliability of the simulation results. The parameters of the potential function depend on the physical properties of the material itself, and different potential functions are applicable to different objects. Vashishta potential function is widely used in SiC nanoindentation molecular dynamics simulation research and can successfully describe the behavior of semiconductor and ceramic materials. In this paper, an improved Vashishta potential function is used to describe the interaction of the Si-C system, which can accurately predict the properties of various phases of SiC. The improved Vashishta potential function combines repulsive force, shielded Coulomb force, shielded charge dipole, diffuse interaction, and bond angle energy. The mathematical expression of the improved Vashishta potential function is as follows:

\[
E = -\sum_{i>j} f_{ij} \left[ \frac{V_{ij}(r_{ij}) - (b_{ij} + b_{ji})}{2\lambda (r_{ij})} \right].
\]

\[
E \text{ represents total energy, } V_{ij} \text{ represents potential energy between } i \text{ atoms and } j \text{ atoms, and } f_{ij}(r_{ij}) \text{ represents truncated functions.}
\]

\[
V = \sum_{i<j} V^{(2)}_{ij}(r_{ij}) + \sum_{i,j,k} V^{(3)}_{ijk}(r_{ij}, r_{ik}),
\]

where \(V\) represents the total energy of the system, \(V_{ij}\) represents the two-body potential energy, and \(V_{ijk}\) represents the three-body potential energy. The two-body part of the effective potential is denoted as follows:

\[
V^{(2)}_{ij}(r) = \frac{H_{ij}}{r_{ij}} + \frac{Z_{i}Z_{j}}{r} \exp \left( \frac{-r}{\lambda_{ij}} \right) - \frac{D_{ij}}{r} \exp \left( \frac{-r}{\lambda_{ij}} \right) - \frac{W_{ij}}{r^{2}}, r < r_{cij}.
\]

\[
V^{(3)}_{ijk}(r_{ij}, r_{ik}) = R_{ijk}^{(3)}(r_{ij}, r_{ik}) P^{(3)}(\Theta_{ijk}),
\]

\[
R_{ijk}^{(3)}(r_{ij}, r_{ik}) = B_{ijk} \exp \left( \frac{Y}{r_{ij} - r_{a}} + \frac{Y}{r_{ik} - r_{a}} \right) \Theta(r_{ij} - r_{a}) \Theta(r_{ik} - r_{a}),
\]

\[
P^{(3)}(\Theta_{ijk}) = B_{ijk} \frac{\cos \Theta_{ijk} - \cos \tilde{\Theta}_{ijk}}{1 + C_{ijk} \cos \Theta_{ijk} - \cos \tilde{\Theta}_{ijk}}^{2},
\]
3.1. Force-Indentation Depth Curve of Nanoindentation at different Temperatures. The $P-h$ curve of indentation at different temperatures is shown in Figure 2. The $P-h$ curve of the load displacement of the 3C-SiC specimen during the nanoindentation process at a temperature of 10 K is shown in Figure 2(a). The $P-h$ curve showed no obvious rapid load drop during the entire indentation process, and the overall performance was elastic deformation. There was a small fluctuation in the load at $h = 0.22$ nm, but the overall indentation was relatively stable. At $h = 0.53$ nm, the load changes linearly with the depth of the indentation. This phenomenon conforms to the Hertz contact theory [4], but the linear correlation occurs later, and the elastic phase delay occurs.

The load displacement $P-h$ curves of the 3C-SiC specimen during the nanoindentation process at 300 K, 600 K, and 900 K are shown in Figures 2(b)–2(d), respectively. The changing trends of the three $P-h$ curves in the indentation process are roughly the same, which proves the correctness of the load-displacement curve. The three curves can be divided into three stages, namely, the elastic deformation stage, the elastoplastic deformation stage, and the plastic deformation stage. From $h = 0.20$ nm to $h = 0.25$ nm, the load is linearly related to the indentation depth, which is the elastic deformation stage. A pop-in [1] point appears at $h = 0.25$ nm, and the 3C-SiC specimen changes from an elastic deformation stage to an elastic-plastic deformation stage. The initial drop points related to the plastic deformation mechanism appear at the same position on the $P-h$ curve, all at $h = 0.50$ nm. At this time, the 3C-SiC specimens changed from the elastoplastic deformation stage to the plastic deformation stage. The initial drop of plastic deformation is more obvious on the curve, the drop is large, and the difference increases with the increase of temperature. Then, the curve rises rapidly, and the 3C-SiC specimen is in the plastic deformation stage at this time.

As shown in Figure 3, comparing the four temperatures at the end point of the indentation $h = 1.00$ nm, it can be found that the load of the 3C-SiC specimen shows a continuous decrease with the increase of the simulated temperature. Obviously, the increase of the temperature can cause the load-bearing capacity of the material has declined in varying degrees, and the 3C-SiC material exhibits high-temperature softening characteristics. Under 300 K, 600 K, and 900 K, the elasticity, elastoplasticity, plasticity, and load-displacement curve change laws are basically the same. However, as the temperature increases, the load value in the elastic-plastic deformation zone is also higher, and the sudden load drop occurs earlier. This is because the high temperature causes the load in the plastic deformation zone to drop earlier. In the plastic deformation zone, the law is just the opposite. The high temperature causes the load value to decrease. Because the occurrence of dislocations is concentrated in the elastoplastic deformation zone, the load value in the elastoplastic deformation zone is generally higher in the high temperature environment.

3.2. Changes of Matrix Stress Distribution with Indentation Depth at Different Temperatures. As shown in Figure 4, Figures 4(a1)–4(c1) select the stress distribution of 3C-SiC specimens at 10 K temperature, and the indentation depths are 0.50 nm, 0.70 nm, and 0.90 nm. It can be seen from the stress distribution cloud diagram that with the deepening of the indentation, the stress distribution in the indenter area becomes more concentrated, and both the normal stress and the tangential stress continue to increase. This period is accompanied by the generation and evolution of horizontal, cross, and vertical dislocations, as well as the process of elastoplastic deformation. When the indentation depth $h$ is
0.50 nm, the high stress area appears in the contact area between the tip of the indenter and the test piece. When the indentation depth is \( h = 0.70 \) nm, the high stress area expands on the basis of Figure 4(a1), mainly concentrated in the contact position of the indenter and the test piece. When the indentation depth is \( h = 0.90 \) nm, the depth of the

### Table 1: Set the parameters of the model.

| Related parameters                      | Parameter value                     |
|----------------------------------------|-------------------------------------|
| 3C-SiC specimen size                   | 24.00 nm × 17.00 nm × 24.00 nm      |
| Number of atoms of diamond spherical indenter | 1021520                               |
| Number of atoms in 3C-SiC sample       | 115845                               |
| Indentation crystal plane              | (010)                                |
| Indentation temperature                | 10 K, 300 K, 600 K, 900 K           |
| Indentation speed                      | 50 m/s                               |
| Indentation depth                      | 1.0 nm                               |
| Step size                              | 1 fs                                 |

Figure 2: \( P-h \) curve of indentation at different temperatures.
The high-stress zone is deepened, the range is enlarged, and a high-stress zone also appears in the peripheral area of the specimen at the same depth as the contact area. This shows that with the deepening of the nanoindentation, the atoms around the indentation contact area continue to concentrate, which increases the strain and the load, accompanied by the elastoplastic deformation process.

In Figure 4, Figures 4(a2)–4(c2), respectively, correspond to the stress distribution cloud diagrams at the time when the temperature is 300 K, and the displacements in the load-displacement curve are 0.50 nm, 0.70 nm, and 0.90 nm. In the elastic deformation zone at 0.5 nm, the load-displacement curve shows a linear change. At this time, the low-strain zone accounts for the majority, and the dislocation is only the dislocation skeletal stage. At 0.7 nm, in the elastic-plastic deformation zone of the load-displacement curve, a large number of dislocations appear at this time, and horizontal and V-shaped dislocations appear. As the indentation depth increases, the contact between the indenter and the specimen regions, the strain distribution in the high-strain region, the lower-strain region becomes more and more obvious. At 0.9 nm, special phenomena such as fracture appear in the dislocation form at this time. At this time, it enters the plastic deformation zone of the load-displacement curve. As the indentation depth increases, the surrounding strain spreads more and more.

Comparing the strain distribution diagrams at temperatures of 300 K, 600 K, and 900 K, it can be found that the change law of the load-displacement curve is basically the same, and the dislocation form is also basically the same. However, with the increase of temperature, the lower strain area in the high strain area becomes more and more obvious. In the case of the same indentation depth, the strain in the high strain area becomes larger as the temperature increases. It can be seen that the temperature rise makes the high strain area more and more obvious, and the extreme values of the load-displacement curve at different stages are also different.

The degree of dislocation corresponding to the nanoindentation experiment at different temperatures is increasing, and the length of the dislocation is getting longer and longer.

3.3. Analysis of 3C-SiC Nanodeformation Mechanism. Figure 5 selects the indentation deformation area of the 3C-SiC specimens when the indentation depth is 0.60 nm, 0.80 nm, and 1.00 nm at 10 K temperature for analysis. When the indentation depth $h$ is 0.60 nm, the indentation deformation area is more concentrated, and the surface of the deformation area is relatively smooth. In the periphery of the deformation area, a small amount of smaller dislocation nucleation areas is produced, which lays the foundation for the subsequent generation and growth of dislocations. When the indentation depth $h$ is 0.80 nm, the indentation deformation area is shown in Figure 5(b). The 3C-SiC specimen has multiple dislocation loops at the dislocation nucleation, and the dislocation loops are more concentrated and surround the deformation area. In the center, it is surrounded by layers. As shown in Figure 5(c), when the indentation depth $h$ is 1.00 nm, the dislocation ring grows on the basis of $h$ 0.80 nm, and there are many larger "V"-shaped dislocation rings. The growth of dislocation loops almost filled the entire 3C-SiC specimen, and this phenomenon coincides with the characteristics of the compound plastic deformation stage. With the increase of the indentation depth, the dislocation loops of the 3C-SiC specimens gradually formed and grew. The deeper the depth, the greater the number of dislocation loops, the longer the length, and the more complex the distribution. The atoms of the 3C-SiC specimen move along with the growth direction of the dislocation, and its movement can be analyzed according to the change of the dislocation.

When $h$ is greater than 0.56 nm, the 3C-SiC specimen is in the plastic deformation stage during the nanoindentation process. Figure 6 selects the indentation deformation area of the 3C-SiC specimen at the time of 0.60 nm, 0.80 nm, and
1.00 nm at the temperature of 300 K for analysis. As shown in Figure 6(a), when the indentation depth \( h \) is 0.60 nm, the indentation deformation area is concentrated, and there is no obvious dislocation nucleation area in the deformation area, which is no obvious difference from Figure 5(a). When the indentation depth \( h \) is 0.80 nm, the indentation deformation area is shown in Figure 6(b), and the dislocation ring grows at the dislocation nucleation. Compared with Figure 5(b), the number of dislocation loops has been significantly reduced. When the indentation depth \( h \) is 1.00 nm, the dislocation loops of the 3C-SiC specimen continue to grow, forming multiple large dislocation loops. However, the number of dislocation loops is less than that in Figure 5(c), the dislocation exchange distribution is simpler, and the atomic movement inside the 3C-SiC specimen is simpler.

Figure 7 selects the indentation deformation area of the 3C-SiC specimen at the time of 0.60 nm, 0.80 nm, and 1.00 nm at 600 K temperature for analysis. As shown in Figure 7(a), when the indentation depth \( h \) is 0.60 nm, the indentation deformation area is concentrated, and a small amount of dislocation nucleation area is generated around the deformation area. When the indentation depth \( h \) is 0.80 nm, dislocations grow into dislocation loops, the number of which increases slightly compared with Figure 6(b). When the indentation depth \( h \) is 1.00 nm, dislocations grow into dislocation loops, the number of which increases slightly compared with Figure 6(b). The dislocation expansion area is wider, the larger "V"-shaped dislocation loops are more numerous and widely distributed, and the atomic movement inside the 3C-SiC specimen is more complex and diverse.
Figure 8 selects the indentation deformation area of the 3C-SiC specimen at the time of 0.60 nm, 0.80 nm, and 1.00 nm at 900 K temperature for analysis. As shown in Figure 8(a), when the indentation depth $h$ is 0.60 nm, the deformation of the indentation is similar to that of Figure 7(a). When the indentation depth $h$ is 0.80 nm, the growth rate of dislocation loops is significantly faster than that in Figures 6(b) and 7(b). The length of the dislocation loop is larger, but the number of dislocation loops is less than that in Figure 5(b). The dislocation growth situation is simpler. When the indentation depth $h$ is 1.00 nm, the indentation deformation area is shown in Figure 8(c), and the dislocation loop distribution is more complicated than that in Figures 6(c) and 7(c). The number of “V”-shaped dislocation loops is larger, and the dislocation extension area is wider and deeper. Similar to Figure 5(c), the dislocation ring
almost fills the entire 3C-SiC specimen, and the distribution is more extensive. The atomic motion inside the 3C-SiC specimen is the most complex and diverse.

4. Conclusion

(1) By simulating 3C-SiC nanoindentation simulation experiments at different temperatures, at 10 K temperature, 3C-SiC is in the elastic and elastoplastic stage. Because the temperature is too low, the 3C-SiC specimen has been destroyed. There is almost no change in the load-displacement curve, directly entering the plastic deformation stage. Under 300 K, 600 K, and 900 K, the elasticity, elastoplasticity, plasticity, and load-displacement curve change laws are basically the same. However, as the temperature increases, the load value in the elastic-plastic deformation zone is also higher, and the sudden load drop occurs earlier. This is because the high temperature causes the load in the elastic-plastic deformation zone to drop earlier. In the plastic deformation zone, the law is just the opposite, and the high temperature causes the load value to drop. Since the occurrence of dislocations is concentrated in the elastoplastic deformation zone, and the load value in the elastoplastic deformation zone is generally higher in a high temperature environment, the stress is also concentrated in the elastoplastic zone, and the energy of the dislocation loop is released. Therefore, in the plastic deformation zone, the premature release of energy due to the fracture of the dislocation loop in the high temperature environment is lower than the load value in the low temperature environment. With the increase of temperature, the bearing capacity of 3C-SiC material decreases, especially plastic deformation occurs inside the material. Dislocations nucleate and grow from the grain boundaries and expand into the crystal and finally form a ‘U-shaped’ dislocation loop

(2) This conclusion has a certain reference for the reasonable selection of nanoindentation specimen materials according to the temperature environment. There is a certain basis for the proper selection of the temperature environment of nanoindentation according to the extreme value of load in different elastoplastic periods

Data Availability

The (Figure 1 to Figure 8) data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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