Rare Metal Materials and Engineering
Volume 52, Issue 11, November 2023
Available online at www.rmme.ac.cn

Science Press

Cite this article as: Lu Doudou, Li Shan, Tang Kebin, et al. Molecular Dynamics Study on Effect of Ion Implantation on Mechanical Properties of Single Crystal Germanium[J]. Rare Metal Materials and Engineering, 2023, 52(11): 3736-3740. DOI: 10.12442/j.issn.1002-185X.20230236.

ARTICLE

Molecular Dynamics Study on Effect of Ion Implantation on Mechanical Properties of Single Crystal Germanium

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Abstract: To improve the hard and brittle mechanical characteristics of single crystal germanium (Ge), the molecular dynamics (MD) simulation was used to study the mechanism of surface modification on single crystal Ge by ion implantation with three different doses. Results show that the ion implantation causes amorphous phase damage to Ge matrix, and the nano-indentation process shows the lattice evolution. The nano-indentation results reveal that the existence of amorphous phase can reduce the hardness and brittleness of single crystal Ge and enhance its plasticity. Additionally, the degree of amorphous phase damage and the hardness of Ge matrix are related to the ion dose. With increasing the ion dose, the amorphous damage is deepened, and the hardness is decreased.

Key words: nano-indentation; molecular dynamics; ion implantation; single crystal germanium

As one of the infrared optical materials, single crystal germanium (Ge) is widely used to manufacture various optical devices, such as infrared lenses and infrared detectors[1], because of its excellent electro-optical properties. Ge is a hard and brittle material, which is usually processed by grinding and polishing[2]. However, these methods can hardly machine the surfaces with complex contour, the processing precision cannot satisfy the current requirements. Besides, the low efficiency and high cost of these methods also restrict their application. Although the single-point diamond turning has become a commonly used method for ultra-precision cutting of hard and brittle materials, the cutting forces are significantly different along different crystal directions, which leads to brittle fracture and cannot achieve high-quality surfaces.

Miao et al[3] proposed the criteria for chip removal modes during the cutting process of single crystal Ge. Yang et al[4–5] investigated the mechanical properties and indentation size effect of different crystal planes of single crystal Ge through nano-indentation experiments. Liu et al[6] suggested that the single crystal Ge undergoes three deformation stages during the loading process: elasticity, plasticity, and brittleness.

Pelaz et al[7] presented the amorphization mechanism of ion implantation on silicon. Guo et al[8] used molecular dynamics (MD) simulation to study the effect of amorphous layer thickness on nano-cutting of single crystal Ge. Results show that the material plasticity is increased with increasing the amorphous thickness. Fang et al[9] proposed the nano-metric machining of ion implanted materials. It is reported that the ion implantation can soften the surface of hard and brittle materials, such as monocrystalline silicon, and increase the brittle-ductile transition depth (BTDT). Chen et al[10] simulated the nano-indentation processes of modified and unmodified monocrystalline silicon, and found that the ion implantation can reduce the hardness of silicon surface and improve the plasticity. Wang et al[11] conducted the copper ion implantation experiments on single crystal Ge and revealed that BTDT of single crystal Ge is significantly increased after copper ion implantation. Fan et al[12] studied the formation mechanism and damage evolution process of silicon vacancy color centers during the annealing process of 4H-SiC material which was implanted with helium ions and double ions.

Ion implantation technique can be used for various hard and brittle materials, but it is rarely used for single crystal Ge. Therefore, in this research, the influence of different doses of ion implantation on the mechanical properties of single crystal Ge was investigated through MD analysis. The relationship between ion dose and amorphous damage was analyzed by visualization software (ovito). In addition, the nano-

Received date: April 24, 2023
Foundation item: National Natural Science Foundation of China (51765027)
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indentation simulations were conducted, and the results demonstrate that the ion implantation can improve the mechanical properties of single crystal Ge.

1 MD Simulation

1.1 Simulation model

Large-scale atomic/molecular massively-parallel simulator (LAMMPS)[13] software was used for simulation. Lai et al[14] studied the phase transition behavior of single crystal Ge during the indentation process by MD simulation. Kosai et al[15] conducted the multi-cycle indentation experiments on single crystal Ge under different loads to study the phase transition behavior. In this research, a three-dimensional model was adopted, as follows:

1) The workpiece was single crystal Ge and it was split into three layers along *Z*-axis direction: boundary layer, thermostat layer, and Newton layer. The periodic boundary condition was adopted along *X*-axis and *Y*-axis directions. *Z*-axis direction was set as the fixed boundary condition.

2) The atoms of boundary layer were neglected in the calculation of time integral and load in order to preserve stationary, therefore decreasing the boundary effects. To dissipate the heat from system, the thermostat layer was maintained at 300 K. The motion of the atoms of Newton layer followed the Newton's second law.

3) Fig. 1 shows the three-dimensional MD simulation model, whose size was 16.971 nm×16.971 nm×28.285 nm.

The schematic diagram of ion implantation simulation model is shown in Fig. 1a. The size of the ion implantation area was 7 nm×7 nm, and the implanted ions were randomly distributed on the model and vertically implanted. This simulation focused on the structural damage caused by implanted ions to the matrix. Thus, the implanted ions were electrically neutral. To achieve sufficient modification, heavy ions are preferred as modification particles. Therefore, the heavy ion Ge was selected as the implanted ion in this research, and the implantation energy was 5 keV. In this case, the implanted ions could cause structural damage to the substrate through cascading collisions. The simulation time step was 1 fs. Three different ion doses (1.0×10^{13}, 2.5×10^{13}, and 6.25×10^{13} ion/cm^2) were chosen for simulation. Fig. 1b shows the schematic diagram of nano-indentation model. The spherical indenter was composed of carbon (C) atoms, and it could be regarded as a rigid body. The material is single crystal Ge and the related simulation parameters are presented in Table 1.

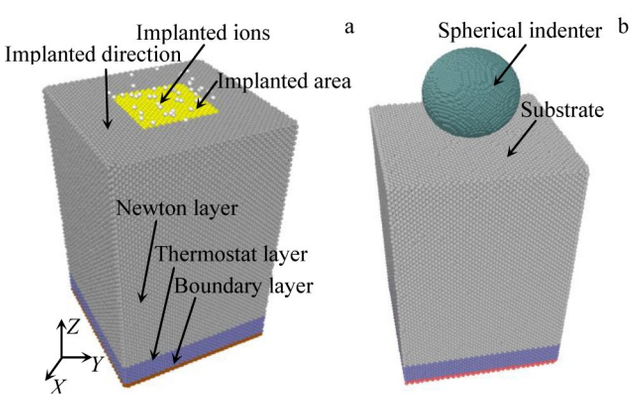

Fig.1 Schematic diagrams of 3D simulation models of ion implantation (a) and nano-indentation (b)

1.2 Simulation potential function

In this simulation, there were three types of atomic interactions: (1) interactions between the workpiece atoms; (2) interactions between the workpiece atoms and implanted ions; (3) interactions between workpiece and spherical indenter. Firstly, Tersoff potential[16] was chosen to describe the atomic interaction between the single crystal Ge atoms in the substrate and that between the implanted ions and Ge atoms in the workpiece. For the interactions between workpiece and indenter, Morse potential[17] was selected to calculate the interaction force. The related parameters of Morse potential are listed in Table 2. Because the spherical indenter was considered as a rigid body, the interaction force between C atoms could be neglected.

2 Results and Discussion

2.1 Ion implantation process

Implanted ions with specific energy can hit the material surface at a certain initial velocity, as shown in Fig.2.

The collision can be caused just after the implanted ions come into contact with the substrate or enter the substrate, resulting in the defects, such as clusters and vacancies in the substrate. Cascade collision leads to energy exchange, and the energy of implanted ions gradually decreases to zero and eventually stays inside the substrate. Ge atoms in the matrix can gain energy by the collision, therefore causing more damage. The depth and degree of the modified layer are related to the type of implanted ion, ion energy, ion incident angle, ion dose, and the properties of matrix material, which

Table 1 Simulation conditions and parameters

Parameter	Value
Workpiece size	16.971 nm×16.971 nm×28.285 nm
Implantation energy/eV	5000
Implantation ion dose/$\times10^{13}$ ion·cm^{-2}	1.0, 2.5, 6.25
Implantation direction	(100)
Indenter radius/nm	4
Loading depth/nm	4
Loading speed/m·s^{-1}	50
Initial temperature/K	300

Table 2 Simulation parameters of Morse potential

Atomic interaction	Parameter	Value
Ge-C	Cohesion energy, D/eV	0.125 78
	Elastic modulus, α/nm^{-1}	25.821 90
	Equilibrium distance, r_0/nm	0.223 24

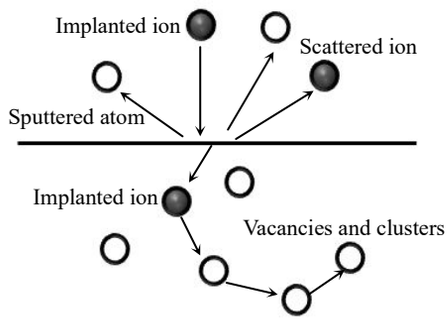

Fig.2 Interaction between implanted ions and matrix

can be adjusted to satisfy the modification requirements.

2.2 Ion implantation damage

Due to the cascade collision generated by implanted ions, the matrix particles are displaced, resulting in point defects, dislocations, and other damages. It is reported that the ion implantation depth is possibly related to the ion energy. The injection depth is roughly proportional to the injection energy, i. e., the greater the energy, the deeper the injection depth. Fig. 3a – 3c show the amorphous clusters defect under three different ion doses. The defect atoms are displayed by reducing the atomic radius of normal Ge through ovito software. Fig. 3d – 3f show the cross-section morphologies corresponding to Fig.3a–3c, respectively.

According to Fig. 3, the implanted ions can introduce defects, such as clusters, inside the substrate due to the random cascade collision of particles. Besides, with increasing the implanted ion dose, the number of defect atoms and the amorphous degree are increased. On the contrary, the proportion of perfect single crystal structures is decreased with increasing the implanted ion dose. The material surface is completely amorphous when the injection dose reaches a certain level. Considering that the ions are randomly implanted, the defects can be uniformly distributed. Therefore, the mechanical properties of Ge substrate caused by the implanted ions are also uniformly changed.

2.3 Nano-indentation simulation

Nano-indentation MD simulations were conducted on modified and unmodified single crystal Ge. Considering the model size, the radius of the selected spherical indenter is 40 nm, and the indentation depth is 40 nm. It is reported that the indentation speed is generally 1–100 m/s in simulation, which is different from the actual experiment speed. The selected indentation speed is 50 m/s in this simulation.

The indenter is regarded as a rigid body, so the force between C and C atoms is neglected during the simulation process. The Morse potential was used to calculate the loading force imposed by workpiece atoms on a spherical indenter. Before simulation, the spherical indenter was located above the model with a certain distance, and then it quickly moved to the plane with the distance of 0.2 nm above the substrate surface. After sufficient relaxation of the matrix material, the indenter was pressed into the matrix at a fixed speed until the depth reached 4 nm.

Fig. 4 shows the morphologies of initial damage, damage propagation, and final damage of unmodified and modified Ge

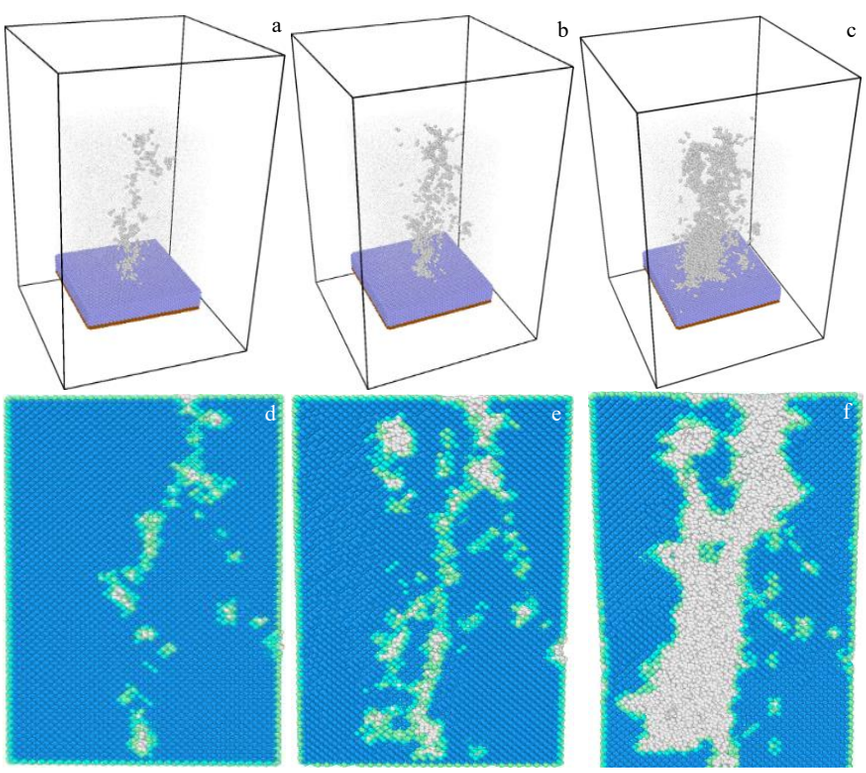

Fig.3 3D (a – c) and cross-sectional (d – f) morphologies of matrix after ion implantation with different ion doses: (a, d) 1.0×10^{13} ion/cm^2; (b, e) 2.5×10^{13} ion/cm^2; (c, f) 6.25×10^{13} ion/cm^2

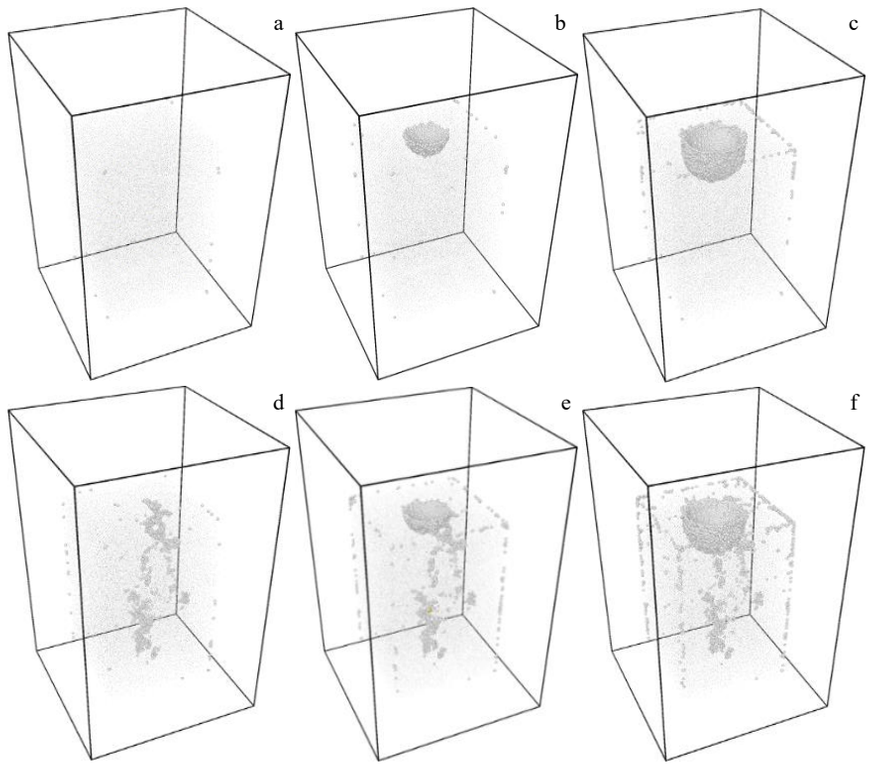

Fig.4 Morphologies of unmodified (a – c) and modified (d – f) Ge during nano-indentation simulation under ion dose of 1.0×10^{13} ion/cm^2: (a, d) initial damage; (b, e) damage propagation; (c, f) final damage

during the nano-indentation simulation. To investigate the mechanism of amorphous formation in the nano-indentation process, the normal atomic radius is reduced and adjusted to facilitate the visual analysis.

During the indentation process, the indenter exerts hydrostatic pressure on the workpiece. With increasing the indentation depth, the hydrostatic pressure is increased. It is known that when the hydrostatic pressure exceeds a certain value, the lattice slip occurs, and the crystal begins to undergo the amorphous phase transition. The atoms around the indenter become disordered, as shown in Fig.4a–4c.

At the beginning of nano-indentation for modified Ge, the amorphous structure damage caused by ion implantation leads to the disordered arrangement of Ge atoms and the internal structure loose. Therefore, during the nano-indentation process, these damages can effectively absorb the hydrostatic pressure induced by the indenter, thereby effectively preventing the lattice distortion. Fig.4d–4f show the structural changes in modified Ge. Thus, it can be concluded that the modified Ge can effectively soften the material surface, reduce the hardness, and improve the plasticity.

The load-displacement curves of nano-indentation process are shown in Fig.5. When the pressure depth is the same, the loading force required for modified Ge of different ion doses is decreased with increasing the ion implantation dose. Therefore, after ion implantation, the hardness of single crystal Ge is reduced, and the mechanical properties are improved. The larger the ion dose, the smaller the required loading force, indicating that with increasing the ion dose, the

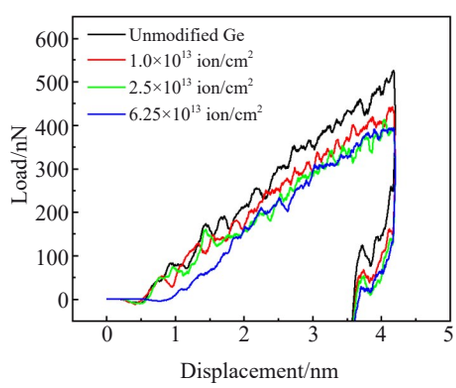

Fig.5 Load-displacement curves of nano-indentation process under different ion doses

lattice transition from regular arrangement to amorphous state is intensified. The improvement in mechanical properties is also obvious. According to the load-displacement curves, it can be concluded that the displacement discontinuity (pop-out) trend weakens, suggesting that the plasticity of modified Ge improves, the brittleness decreases, and the probability of crack occurrence becomes less, which is beneficial to improve the surface quality.

3 Conclusions

1) Ion implantation on single crystal Ge matrix can result in the cascade collision between particles and matrix atoms, which causes lattice damage of a certain depth and leads to

amorphization.

2) The amorphization degree of single crystal Ge is related to the implantation ion dose: with increasing the ion dose, the amorphization degree is increased correspondingly.

3) The mechanical properties of single crystal Ge can be improved by ion implantation. The hardness is decreased and the plasticity is increased with increasing the ion dose.

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离子注入对单晶锗力学性能影响的分子动力学研究

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摘　要：为改善单晶锗的硬脆力学特征，用分子动力学模拟方法研究了3种不同剂量的离子注入对单晶锗表面的改性机理。分析结果表明，离子注入对锗基体造成了非晶相损伤，纳米压痕过程表现为晶格演化。纳米压痕结果揭示了非晶相的存在能够降低单晶锗的硬度和脆性，提高塑性。此外，锗基体的非晶相损伤程度和硬度与离子剂量有关。随着剂量的增加，非晶损伤程度加深，硬度降低。

关键词：纳米压痕；分子动力学；离子注入；单晶锗

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