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The tensile effect on crack formation in single crystal silicon irradiated by intense pulsed ion beam

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ABSTRACT

Improving antifatigue performance of silicon substrate is very important for the development of semiconductor industry. The cracking behavior of silicon under intense pulsed ion beam irradiation was studied by numerical simulation in order to understand the mechanism of induced surface peeling observed by experimental means. Using molecular dynamics simulation based on Stillinger Weber potential, tensile effect on crack growth and propagation in single crystal silicon was investigated. Simulation results reveal that stress-strain curves of single crystal silicon at a constant strain rate can be divided into three stages, which are not similar to metal stress-strain curves; different tensile load velocities induce difference of single silicon crack formation speed; the layered stress results in crack formation in single crystal silicon. It is concluded that the crack growth and propagation is more sensitive to strain rate, tensile load velocity, stress distribution in single crystal silicon.

1. Introduction

For the development of material with high resistance to radiation damage or with exotic properties produced by atomic-level modification, it is important to analyze the structural deformation when intense pulsed ion beam (IPIB) bombards the materials. IPIB as an inertial fusion driver is firstly used in fusion research [1]. Based on energies of hundreds of keV, ion currents from 1 kA to MA and pulse length of tens to hundreds ns, IPIB has been utilized for various surface treating applications such as surface hardening [2–4], ablation [5,6], wear and corrosion resistance improving [7], film deposition [8,9], nanopowder synthesis [10], and so on [11]. Applications of single crystal silicon in semiconductor industry, such as integrated circuit, solar cell, micro-electro-mechanical systems (MEMS), have grown in recent years. However, it is very difficult to clarify the deformation process of silicon irradiation by IPIB, which is a nonequilibrium transient process. Therefore, computer experiments are regarded as a powerful tool to get complementary insights in real experiments. Molecular dynamics (MD) simulation which is a useful tool to analyze microstructure of materials has been widely used to investigate the fundamental mechanism of mechanical properties of silicon on micro scale.

There are many research literatures related to IPIB induced material deformation by using MD simulation. Y. Sasajima and coworkers have analyzed the structural relaxation caused by IPIB irradiation of single crystal silicon, the supplied thermal energy was first spent to change the crystal structure into an amorphous structure within a short period of about 0.3 ps, then it diffused in the specimen by an ordinary thermal dissipation process [12]. The thermal expansion coefficient and lattice constant of bulk silicon have been obtained using different potentials and results indicate that Stillinger Weber (SW) potential has a better agreement with the experiment observations [13]. An atomic model of single crystal tungsten containing a pre-existing crack was built, and crack propagation behavior with and without hydrogen atoms under uniaxial tensile load was investigated, high hydrogen concentration could result in rearrangement of tungsten atoms ahead of the crack tip and reduce the stress concentration in the neighboring area around the crack [14]. The tensile stress-strain curves of single crystal tungsten nanowire and its microscopic deformed structures at different temperatures were simulated by MD method, results showed that the stress-strain curves could be all divided into five stages: elastic, damage, phase transition, hardening and failure stages [15]. Tungsten ablation under IPIB irradiation, mechanical behavior of single crystal copper,

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crack growth and propagation of single crystal nickel, defect size were investigated by using MD simulation [16–19].

However, there is short of study on single crystal silicon crack formation after IPIB irradiation. The mechanical properties of silicon are influenced by defects such as cracks, vacancies, dislocations, and so on [20,21]. Since defects occur across several different microscopic scales, it is very difficult to verify the mechanism of crack formation using direct experimental methods. Fig. 1 shows crack formation on the surface of single crystal silicon irradiated by IPIB for 50 pulses, the irradiation experiment was performed on the TIA-450 accelerator at College of Materials Science, Shenyang Ligong University. The beams from the accelerator were mainly composed of 70% C^{n+} and 30% H^{+}, and the ion source was provided by magnetic insulate diode of graphite anode. Typically, the peak values of accelerating voltage and current density were 350 kV and 130 A/cm^2, respectively. The pulse duration was 60 ns. The arrow indicates one of cracks grows along straight line in Fig. 1. In this paper, in order to investigate the mechanism of crack growth and propagation, MD simulation method was used to study stress-strain curves, tensile load velocity and stress distribution in single crystal silicon.

2. Simulation method and atomistic model

In this work, MD simulations were adopted to analyze tensile effect on single crystal silicon by using the Large-scale atomic/molecular massively parallel simulation (LAMMPS) software [22]. The three dimensional MD model of single crystal silicon is shown in Fig. 2. The model is diamond structure with cuboid geometry. The model size is 50a × 20a × 2a, where a is the lattice constant of silicon and taken as 5.431 Å. The specimen containing 16,200 atomic positions has a dimension of 27.155 nm, 10.862 nm and 1.086 nm in X, Y, and Z directions, respectively. Periodic boundary condition is imposed in X, Y, and Z directions. The interatomic potential plays an important role in MD simulations. One of the widely used potentials for silicon is SW potential [23], which considers a linear combination of two and three body terms to express the cohesive energy. To eliminate the nonequilibrium of potential energy and local stress, the specimen is relaxed 20 ps within isothermal-isobaric ensemble to its equilibrium configuration. The other parameters including temperature of 300 K and pressure of 0 Pa are imposed in the MD equilibrium configuration.

In order to observe crack formation in single silicon, which is irradiated by IPIB, we calculate following procedures: loading a constant strain rate to the specimen, loading a constant velocity to special atoms, and calculating stress distribution in the specimen. The open visualization tool (OVITO) [24] code is used to quantitative measure the morphology of crack formation in single silicon.

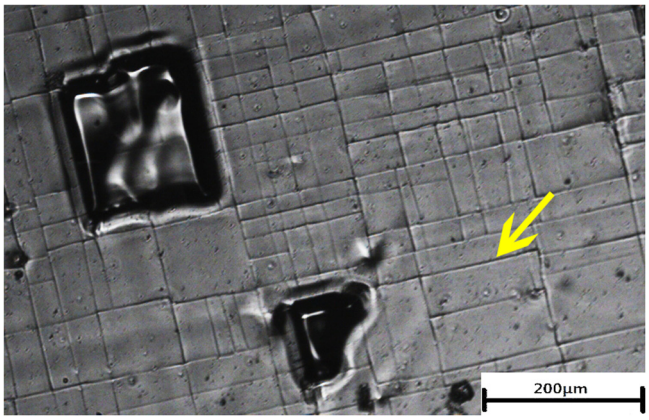

Fig. 1. SEM image of single crystal silicon irradiated by IPIB under 350 keV ion energy and 130 A/cm^2 current density for 50 pulses.

3. Results and discussion

The influence of irradiation on single crystal silicon was firstly studied by comparing the stress-strain curve differences between X, Y, and Z direction. Since irradiation induces material deformation in a transient process, the tensile load is applied in a constant strain rate. The given strain rate is 1.0×10^{10} s^{-1}. According to crack mode I [25], we assume that the direction of crack propagation is X axis direction, which is arrow direction in Fig. 1. Therefore the direction of tensile stress inducing crack propagation is along Y axis direction. Uniaxial strain is applied to the irradiated single crystal silicon, the obtained stress-strain curves are given in Fig. 3. In Y direction, the stress increases with increase of strain until reaching a critical point, then the single crystal silicon yields with decrease of stress. AB stage is silicon elastic deformation process, the relationship between stress and strain is linear relation. When strain exceeds 20%, the stress-strain relationship quickly becomes nonlinear. In BC stage, the stress value is sharp decline from 17.19 GPa to 4.49 GPa. We consider BC stage may involve covalent bond fracture. The stage is different from metal deformation that has a yield process. The stress is barely fluctuated in CD stage, but the stress value is about 4 GPa with increase of strain,

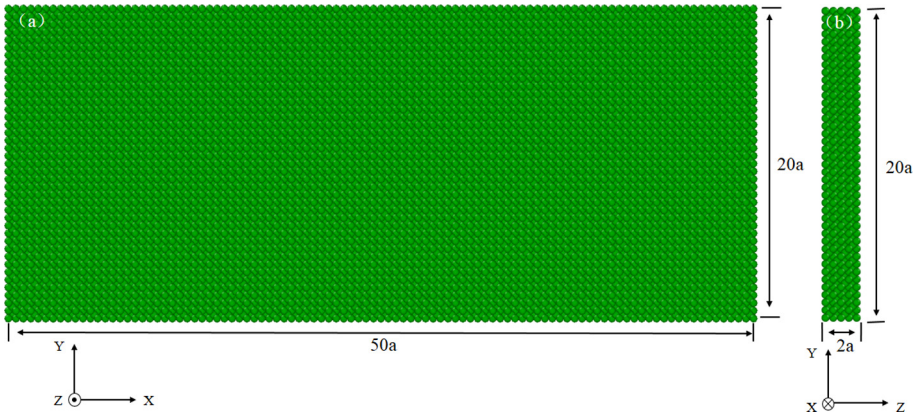

Fig. 2. Atomistic configuration of single crystal silicon in MD simulation (green dots represent silicon atoms) (a) front view of atomic specimen in X-Y plane, (b) side view of atomic specimen in Y-Z plane. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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