Silicon Lattice With Single Vacancy

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Contributor: Feng Dai

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Keywords: silicon ; defects ; molecular dynamics ; mechanical properties

1. Overview

The effect of vacancy defects on the structure and mechanical properties of semiconductor silicon materials is of great significance to the development of novel microelectronic materials and the processes of semiconductor sensors. In this paper, molecular dynamics is used to simulate the atomic packing structure, local stress evolution and mechanical properties of a perfect lattice and silicon crystal with a single vacancy defect on heating. In addition, their influences on the change in Young's modulus are also analyzed. The atomic simulations show that in the lower temperature range, the existence of vacancy defects reduces the Young's modulus of the silicon lattice. With the increase in temperature, the local stress distribution of the atoms in the lattice changes due to the migration of the vacancy. At high temperatures, the Young's modulus of the silicon lattice changes in anisotropic patterns. For the lattice with the vacancy, when the temperature is higher than 1500 K, the number and degree of distortion in the lattice increase significantly, the obvious single vacancy and its adjacent atoms contracting inward structure disappears and the defects in the lattice present complex patterns. By applying uniaxial tensile force, it can be found that the temperature has a significant effect on the elasticity–plasticity behaviors of the Si lattice with the vacancy.

2. Background

With the continuous reduction in the chip size of microelectronic devices with high-cost performance, higher requirements have been proposed for the processing of materials used in these devices. Since the concept of micromachining based on silicon materials was proposed in the 1970s, it has been the key to technological breakthroughs of the microelectromechanical system (MEMS) for the fabrication of micromovable structures based on silicon materials employed by micromachining technology, which are compatible with integrated circuits, for manufacturing microsystems [1]. Especially in the recent decades, the rapid developments of the internet, unmanned driving, wise medical and smart robots have provided unlimited possibilities for applying MEMS sensors in microelectronic devices [2][3][4][5][6][7][8][9].

MEMS is a miniaturized device or a combination of these devices. This system integrates electronics, machinery, optics and other functions to achieve intelligent effects in minimal space. In order to achieve these effects, a breakthrough in the manufacturing technology is required. When the size of a MEMS device is reduced to a certain range, they show many physical phenomena that are different from those in macroscopic systems. For example, the tensile testing data present distinguished differences for the millimeter and micrometer samples [10]. When the size or the spacing between units is within 1 μm or less, the processing technology for these three-dimensional devices is called micromachinery. As micromachining was originally developed from silicon microelectronics processing technology, it is also called silicon-based micromachining [11][12].

As the most important semiconductor material, crystalline silicon has a diamond structure and covalent bonds among atoms. It has excellent mechanical properties, such as high strength and high hardness, as well as good thermal conductivity. Meanwhile, it also has excellent characteristics in light, heat, electricity, magnetic and other properties, and thus can be integrated into capacitive sensors, thermoelectric light detectors, hot gas pressure sensors, magnetometers and photoelectric monitors [13][14][15][16][17][18]. In these MEMS devices, there are many Si wafers, which are flat or have different shapes, including beams, bridges and probe arms. They can be used as light-conducting devices for optical communication, grating devices, micronozzles, microvalves, pumps, micropipes, etc. [19][20]. Moreover, non-linear cantilever, small arc parts, etc., appear in MEMS microsensors, such as tactile sensors on the robot manipulators and chemical reaction sensors [21]. These silicon wafers with different shapes and structures need to be plastic processed.

However, the fracture strength of silicon is very low. Various observation approaches give values of tensile fracture strength in the range of 3 to 7 GPa [22][23]. In addition, early loading experiments with a bearing ball on mirror-polished silicon wafers yield an average fracture stress of 2.8 GPa and a maximum value of 6.9 GPa [24]. The transition from elasticity to plasticity occurs only when the temperature exceeds 790 K. When the temperature is above 920 K, the plastic forming becomes easy [25][26]. At the end of the last century, J. Frühauf et al. [25][26] proposed a laser technology to make materials plastically bend. When laser beams scan the silicon-based surface, plastic deformation occurs owing to the fact that non-uniform temperature field generates thermal stress in the materials [27]. The defects in the silicon bulk greatly affect the forming process. Vacancies and interstitial atoms are the two most important primary point defects in silicon single crystals [28]. Some silicon atoms can remove the binding of the surrounding atoms and jump away from the equilibrium position to form vacancies under specific conditions. Subsequently, the atoms entering the lattice spaces become interstitial atoms [29]. These vacancies can trap the carriers in the silicon crystal by generating deep energy levels, resulting in a decrease in the number of carriers, and affect the performance of semiconductor devices [30]. This kind of defect is not only related to the formation of other forms of defects, but also controls the diffusion of interstitial atoms in semiconductors. At the same time, the existence of the vacancies provides greater possibilities for material deformation [31]. Therefore, it has always attracted attention from experimental and theoretical researchers [32][33]. In the laser bending process, the silicon absorbs the energy from the laser irradiation, so as to produce an uneven transient temperature field in the material matrix. When the temperature of the material surface rapidly increases, the heat generated by the laser diffuses into the material. This additional energy results in changes in the configurations and numbers of defects inside the matrix, and eventually changes the mechanical properties of the crystal. As the heating process is only controlled by the macrotemperature field in the experiment, it poses great difficulties in observing and measuring the changes in the microstructure and mechanical properties in the matrix containing vacancy defects under the conditions of rapid heating by high-energy laser irradiation. Thus, computer simulation based on the empirical potential, such as molecular dynamics, has become a powerful tool to study atomic movements, packing evolution and stress distribution.

The Stillinger–Weber (SW) potential [34] is composed of two-body and three-body potential functions. It can give the strain energy in a few potential parameters and can be used to describe many kinds of defects in silicon. At present, the SW potential function has been successfully applied in studying vacancy defects [35]. In this paper, the molecular dynamics method based on the SW empirical potential [34] of the interaction among atoms in silicon crystalline was used to simulate the heating process of silicon crystal with single vacancy and analyze the packing structures, atomic localization, stress and Young's modulus of the crystal change with temperature.

3. Conclusions

The simulation results show that the silicon lattice has obvious elasticity, elasticity–plasticity transition and plasticity temperature ranges. The existence of the vacancy significantly reduces the elasticity–plasticity transition temperature and greatly affects the mechanical properties of the silicon lattice. In the elastic temperature range, the Young's modulus with the vacancy is lower than that of a perfect lattice. With the increase in temperature, the vacancy migrates, which leads to the change in stress distribution in the region of its nearest neighbor atoms. As the distance between atoms increases largely, the atoms leave their equilibrium positions, and the lattice loses its elasticity, causing the silicon with the vacancies to show plasticity; correspondingly, the Young's modulus of the lattice with a vacancy in the plastic temperature range significantly fluctuates. In the temperature range of elasticity–plasticity transition, the Young's modulus of the lattice is anisotropic. At 1500 K, the single vacancy and shrinkage of its neighboring atoms disappear obviously, and the crystal lattice is distorted greatly. With a further increase in temperature, the defects in the crystal lattice show a complex pattern, and the number of atoms under high pressure increases obviously. The temperature significantly affects the mechanical behavior of the silicon lattice with a vacancy. The elongation of the lattice decreases during the heating process. In the temperature range in which plastic deformation occurs, the tensile strength of the lattice decreases. Due to the existence of the vacancy, the elastic and plastic behaviors present apparent differences with the increase in temperature.

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