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The role of point defects in the swelling and elastic modulus of irradiated cubic silicon carbide

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ABSTRACT

A molecular dynamics study has been performed to investigate the role of point defects in volumetric swelling and elastic modulus of irradiated 3C-SiC in the low and intermediate temperature regime. It is found that different kinds of point defects have distinctive effects on the swelling and Young's modulus. The vacancies have the negligible influence on volumetric swelling while significant on the Young's modulus. However, the value of volumetric swelling and the change in Young's modulus due to the formation of other point defects vary with defect concentration exponentially which we are interested. Furthermore, it is indicated that the relation of the swelling of 3C-SiC and the contribution of point defects is independent on the temperature. During the tensile test, however, the role of carbon interstitial in Young's modulus would be enhanced by temperature. Finally, an approximate model to estimate the antisite defect concentrations in irradiated 3C-SiC is presented.

1. Introduction

The excellent physical and chemical properties of silicon carbide (SiC) make it an attractive candidate for a variety of applications, including the structural component in fusion reactors [1] and high-temperature reactors (HTR) [2], and the fuel cladding material for gas-cooled fission reactors [3] and supercritical water-cooled reactor (SCWR) [4] as well as the advanced electronic devices [5]. Ion-implantation doping and various irradiations inevitably induce the atomic defects, lattice disorder, and even amorphization in 3C-SiC [6–10], affecting not merely the physical properties of β-SiC, but the mechanical performance of SiC-based components as well. Therefore, it attracts a large number of experimental and theoretical efforts.

The irradiation-induced swelling of SiC has been well experimentally studied for the low and intermediate temperatures (~293–1273 K) [3,11–17]. It is found that the amorphization of SiC (a-SiC) would lead to a substantial volumetric expansion of 10.8–12.6% [11]. Snead et al. [3] reported that for the temperature regime between 423 K and 1073 K, referred to the point defect swelling regime, the swelling increases with neutron dose until it approaches saturation, with a steady decrease in the saturation swelling level as the increasing of irradiation temperature. Neutron irradiation experiment performed by Yano et al. [16] showed that the critical temperature for loop formation lies between 753 K and 793 K in the case of 28 dpa. They also reported that the formation of point defects is the main reason for the swelling at the low irradiation temperature even in the case of very high irradiation dose condition. However, both of them did not take into account the role of different kinds of point defects in volumetric swelling of SiC. Li et al. [18] studied the influence of different kinds of point defects in 3C-SiC on the variation of volume by introducing one point defect into the sample at 0 K using molecular static (MS) method. But the influence of thermal vibration and concentration of point defects on the swelling has not been considered, and the mechanism of the influence of point defects on volumetric swelling is limited.

In addition to the swelling, information regarding the influence of point defects on mechanical properties of 3C-SiC is also important. It is worth to note that for the a-SiC, there is a significant decrease in the mechanical properties such as hardness and elastic modulus by 20–60% and 25–45%, respectively [19,20]. By using the Tersoff potential, an estimation of the influence of lattice relaxation on elastic modulus has been performed, indicating that a linear lattice swelling of 1% causes approximately 10% reduction in elastic modulus [3]. From the RBS/C and XRD experimental investigations, Debelle et al. [21,22] reported that in the low dose range (up to ~0.2 dpa), small interstitial-type defects play an important

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role in the production of tensile strain which will stimulate the formation of amorphization at higher dose. But due to the limitation of these experimental techniques, they cannot confirm whether vacancy-type and antisite-type defects would affect the strain field or not. Moreover, Gao et al. [10] studied the variation of the elastic constants as well as the bulk and elastic moduli of SiC with increasing dose at 300 K using molecular dynamics simulation. They reported that these changes began to saturate at doses greater than 0.1 dpa, indicating that point defects and small clusters contribute more significantly to the changes of elastic constants than the topological disorder associated amorphization. By using molecular dynamics at room temperature, Niu et al. [19] investigated the influence of chemical disorder on the mechanical properties. It was suggested that the accumulation of chemical disorder plays a significant role on the decrease in Young's modulus and strength. To date, however, the contribution of each kind of point defects to elastic modulus in irradiated SiC is less understood both from experimental and simulation results.

In this work, we investigate the role of different kinds of point defects in volumetric swelling and elastic modulus of irradiated 3C-SiC at low and intermediate temperatures. Meanwhile, the relationship between the point defect concentration and the considered properties of 3C-SiC is analyzed. On the basis of these results, an approximate model to estimate the antisite defect concentrations in irradiated 3C-SiC is made.

2. Modeling methods

The atomic interactions with a hybrid Tersoff/ZBL potential, which was obtained by modifying the Tersoff potential [23] to improve the description of property of close-separation pairwise, are described with Tersoff potential parameters [24]. The potential has been known to describe adequately the crystalline and amorphous phases of SiC. Moreover, this potential has been successfully employed in many atomistic simulation studies in the past, such as axial compression and tension of 3C-SiC nanowires [25–27], mechanical properties of crystalline, nanocrystalline and amorphous SiC [19,28,29], irradiation-induced point defects in single crystal 3C-SiC [6,7,10,30,31] and nanocrystalline SiC [29,32–35]. In order to make it properly describe the properties under large strains, Tang et al. [36] modified the potential using variable cutoffs to study elastic and thermal properties of SiC and brittle fracture of SiC under hydrostatic pressure. However, Wang et al. [26] tested several cases using the same technique, and they found that there was no difference using the potential without adjusting the cutoffs.

All simulations are performed with the LAMMPS computational codes [37]. A constant pressure and temperature ensemble with periodic boundary conditions in all directions is employed. The monocrystalline samples contained 8000 atoms ($10 \times 10 \times 10$ unit cells). In order to determine the role of point defects in the swelling and elastic property of 3C-SiC, different concentrations of point defects with a given type are introduced at random positions in the simulation cell. Defect concentration is defined as the ratio of the number of defects to the total number of atoms in the samples. All of the introduced point defects are constrained to be at a distance of two unit cells away from the boundary to avoid the periodic boundary effect. We consider different types of vacancy and antisite defects, namely, carbon vacancy (V_C), silicon vacancy (V_{Si}), carbon antisite (Si_C), silicon antisite (C_{Si}). Furthermore, we restrict our study to two stable interstitial configurations depending on the formation energy [38]. One is carbon interstitial atom of the C–C<100> dumbbell configuration, in which two carbon atoms share a regular carbon lattice site along <100>. The other is the silicon interstitial atom, Si_{Tc}, which is located at the tetrahedral position surrounded by four regular carbon lattice atoms. The method to define the isolated point defect has been discussed in our previous work [39].

The initial structures are equilibrated for 100 ps with a timestep of 0.1 fs at a given temperature, which allows the simulation box to achieve stable configurations. The maximum defect concentration is constricted to ensure that these introduced point defects are remained as the initial configurations. Then, the samples are loaded in tension along the [100] direction at a constant deformation rate. In order to balance the simulation efficiency and the result accuracy, the strain rate in this work is set to be 10^{-4} ps^{-1}. The normal stresses σ_y and σ_z in the perpendicular directions are fixed at zero. Meanwhile, all the atoms are forced to deform via an affine transformation that exactly matches the box deformation. Each increment of the box length is followed by a relaxation phase of 30 ps to allow a complete decay of transient forces and to obtain a macroscopic equilibrium configuration at the prescribed strain. The elastic portion of the stress–strain ($\sigma - \varepsilon$) curve is used to determine the elastic modulus. Five runs for each kind of considered point defect are performed.

3. Results and discussion

3.1. Perfect SiC crystal

In order to validate our method and provide basic data for the study of the influence of point defect concentration on Young's modulus of 3C-SiC, Young's modulus along the [100] direction of perfect 3C-SiC at different temperatures, derived from the stress–strain curves with the strain less than 3.0%, has been calculated as shown in Fig. 1. It is found that Young's modulus along [100] direction (Y_0) is 473.24 GPa at 300 K, which is well covered in the range of the observed experimental values 392–694 GPa at 300 K [40]. In addition, it is indicated that Young's modulus of 3C-SiC decreases as the temperature increases from 300 K to 1200 K due to the softness of the material [3]. This is consistent with the results of Im et al. [41] that the elastic constants of SiC crystal decreased from about 475–449 GPa by increasing the temperature from 300 K to 1200 K. The increased fluctuant values of Young's modulus in Fig. 1 maybe due to the enhanced atom vibration at high temperatures.

3.2. Volumetric swelling

The volumetric swelling of 3C-SiC at 300 K is depicted as a function of point defect concentration in Fig. 2. Each kind of point

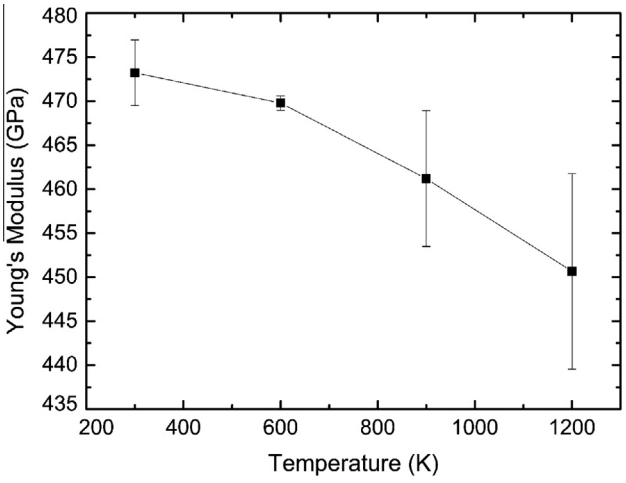

Fig. 1. Temperature dependence of Young's modulus of bulk 3C-SiC.