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Tensile mechanical behaviors of cubic silicon carbide thin films

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ABSTRACT

Molecular dynamics (MD) methods using Tersoff potential are employed to study the nanomechanical behaviors of 3C-SiC (010) thin films under [100]-oriented tension. In this work, the Young's modulus, tensile strength and elongation of thin films are compared with those of the bulk 3C-SiC for different temperatures. The results show that Young's modulus of the nanofilms is size dependent and softer than its bulk counterpart. It is found that Young's modulus decreases as much as 24.7% when the thickness of the thin film reduces to unit lattice, which suggests that size effect could not be neglected when the characteristic length shrinks down to several nanometers. When the thickness of the thin films is more than 10 nm, and thin film value converges to the bulk value. As the increment of thin film value is very slow, the size effects of 3C-SiC could be neglected. In addition, the reduction in Young's modulus of the nanofilm with increasing temperature exhibits a nonlinear trend. Moreover, the simulations demonstrate that the tensile strength and elongation of bulk 3C-SiC also decreases with the increase of temperature. Despite partial degradation, SiC nanofilm maintains its mechanical properties largely at elevated temperatures, which makes it attractive for applications in high temperature environment.

1. Introduction

Silicon carbide (SiC) is a wide band-gap semiconductor, which is a suitable material as building blocks of electronic devices operating at high temperature, high power and high frequency as well as in harsh environments [1]. Among the variety of SiC polytypes, the cubic system (3C-SiC or β-SiC) is the one that presents the most interesting electronic properties. Moreover, 3C-SiC is the only crystal texture that can be epitaxially grown in single crystal form on non-SiC substrates, such as silicon (Si) [2]. Experimentally, crystal 3C-SiC is usually obtained by chemical vapor deposition (CVD), molecular beam epitaxy (MBE) or sputtering, yet this phase cannot be grown as bulk material [3]. Recent advances of SiC growth technology have showed great power in using single crystalline 3C-SiC thin film as a protective coating for Si-based Micro-Electro-Mechanical Systems (MEMSs) [4].

Among thin films of covalent materials, Si has been studied [5–9] most extensively because of its technological importance in MEMS due to its outstanding electronic and mechanical properties in combination with mature processing technologies. However, silicon shows poor performance in applications characterized by high temperature environments. The operating limit of silicon-based transducers containing *pn*-junctions is limited to below 150 °C [10]. For the mechanical properties, the upper limit for silicon-based micromechanical structures is around 500 °C, and silicon surface is chemically active and will appreciably oxidize at temperatures above 800 °C [11]. While some examples are shirt-button-sized gas turbines, postage-stamp-sized rockets, and miniature pressure sensors—all experiencing temperatures of 1000 °C or higher [12]. Thus it requires that silicon-based MEMS structures be enclosed in protective packaging to make them suitable for use in harsh chemicals, oxidizing atmospheres and high erosion conditions, and silicon carbide is the leading candidate as protective packaging. Furthermore, with thermal conductivity three times greater than silicon, it is well suited for coatings in heat exchange applications [13].

Accompanying the emergence of nanotechnology, research effort has been focused on nanotubes or nanowires [14–18]. Understandably, much less effort has been on thin films, because of the difficulty in fabricating these structures [19]. However, it is eventually unavoidable that nanoplates will be present in various nanotechnologies.

Common ceramic products are designed to withstand compression, but MEMS materials must withstand tension to permit a wide range of designs [12]. In contrast to Si, study of the silicon carbide is much less. Lack of precise control over mechanical properties can lead to degradation of nanoscale electronic devices, and therefore it is essential to understand the mechanical properties of SiC nanoplates at the atomistic level. For long-term reliability for practical applications, it is essential to understand the mechanical behaviors of SiC nanoplates including Young's modulus, tensile strength and elongation, etc.

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In nanoscale devices, large stresses will be generated due to thermal or lattice mismatch between different materials. Consequently, the reliability of many devices depends critically on the response of nanostructures to mechanical loading. Several recent studies have examined the influence of 3C-SiC growth conditions on the mechanical properties of the resulting films. It has been shown that the microscopic strain in 3C-SiC films depends on several key factors, including the temperature at which the carbon containing precursor is introduced [20], the construction of the substrate [21] and growth temperature [22]. Under proper conditions, 3C-SiC films can be produced with very low residual stresses without any post-deposition processing. Therefore, if we know the mechanical properties of the 3C-SiC thin films with different thicknesses and temperatures, we can control the growing conditions in order to improve the efficiency of fabricating 3C-SiC thin films.

A number of theoretical calculations have been performed [23–26] to study the mechanical properties of bulk SiC. However, mechanical properties due to quantum size effect in the thin films can be different from those in their macro-counterparts. Atoms at a free surface or interface experience a different local environment than do atoms in the bulk material.

Molecular dynamics (MD) is one of the most fundamental computational techniques used to explore the microcosmic mechanism of deformation and the intrinsic characteristics of a structure at the atomic level, which greatly enhances the understanding realized from experiments. It is widely used for simulating the physical and mechanical properties of various nanomaterials, such as two-dimensional nanoplates [8,9,27]. Molecular dynamics simulations with empirical potentials have been used successfully to provide insights into the mechanical behaviors and deformation mechanisms of SiC.

The purpose of this study is to perform mechanical tensile simulation of 3C-SiC thin films by reporting the elastic modulus, strength, and elongation of the single-crystal material. This article reports the results of MD simulations on the mechanical behavior of 3C-SiC nanoplates. The rest of this article is organized as follows. The next section describes the model and details of the computational method. In Section 3, we discuss the main results, followed by a summary of the principle findings in Section 4.

2. Simulation methods

The atomic interactions were modeled using the 1994 Tersoff potential [28]. In order to make it properly describe the properties under large strains, Tang and Yip [29] modified the potential using variable cutoffs to study elastic and surface properties of 3C-SiC. Further, the Tersoff potential predicted correct surface energy and excellent vertical displacements for (100) surface relaxation. Wang et al. [14] tested several cases using the same technique and found no difference by using the potential without adjusting the cutoffs. Although the first-principles quantum mechanical methods generally give the most accurate results, they cannot be applied to a larger system and longer simulation time. The short-range potentials employed here should not affect the main conclusions obtained in the present investigations and could provide some useful results. What is more, Tersoff potential has been used in many atomistic simulations, such as axial compression and tension of 3C-SiC nanowires [14,15], mechanical properties of crystalline, nanocrystalline and amorphous SiC [30–32].

All MD simulations were performed with the LAMMPS computational codes [33]. A constant pressure and temperature (NPT) ensemble was employed. The initial structures of the thin films were equilibrated for 2.5 ns with a time step of 0.5 fs at a given temperature, which allowed the thin films to achieve stable configurations. The temperature of the system was controlled by rescaling the atomic velocities in every 100 integration steps. The strain was then applied to study the mechanical response of the thin films. At each load step, the system was deformed by multiplying the x-axis length of the simulation box by $1+\varepsilon$, where ε was a very small value, chosen to produce the desired deformation rate $10^8\ s^{-1}$. Meanwhile, all the atoms were forced to deform via an affine transformation which precisely matched the box deformation. The x component of the atomic stress tensor was calculated and averaged over the entire system as a macroscopic tensile stress.

A typical simulation cell of thin films is shown in Fig. 1. A rectangular coordinate system is used with x and z axes along the length and the width directions and the y axis along the thickness direction perpendicular to the thin film surface. One layer thickness is assumed to be a silicon carbide crystal cell with the lattice parameter l; and thus, the model for the SiC plate has N crystal cell layers along the thickness: $N = 1, 2, 3, 4, 5, 8, 12, 25, 40$ layers; and infinite number of layers—that is bulk crystal. The dimensions along x and z directions are both 10 layers long. The number of atoms ranges from 800 to 32000, and the plate thicknesses range from 0.436 to 17.44 nm. Periodic boundary conditions are applied along the two horizontal nanoplate (010). For cubic crystals, the crystal faces (010) and (100) are equivalent. Several atomic layers are removed along the vertical [010] direction to create vacuum regions which are thick enough to avoid interactions between them, so that the top and the bottom of the simulation cell represent two flat free surfaces. Therefore, it is the same as a single plate.

3. Results and discussion

3.1. Potential energies

As shown in Fig. 2, the potential energy decreases exponentially as the thickness of the thin films increases at a given temperature. It suggests that the potential energy decreases quickly first, and then slow down due to the fact that the surface atom percent decreases with increasing thickness. While the surface energy for sufficiently thick plates of ~10 nm becomes constant −6.34 eV/atom,

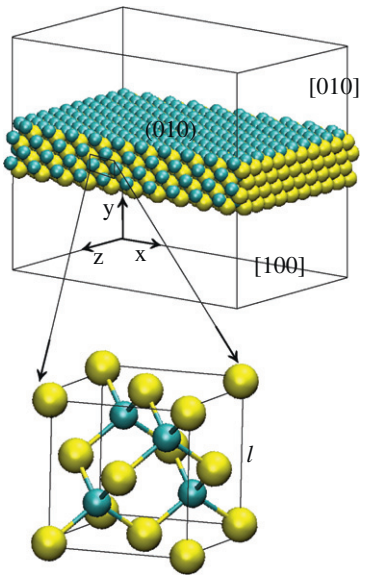

Fig. 1. The 3D model of a (010) silicon carbide thin film. The bigger yellow and smaller blue balls denote the Si and C atoms, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)