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Fracture properties of nanoscale single-crystal silicon plates: Molecular dynamics simulations and finite element method

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ABSTRACT

The thickness- and chirality-dependent mixed-mode I-II critical stress strength factors (SIFs) and crack growth angles of single-crystal silicon (SCS) [1 0 0] and [1 1 0] plates are investigated using molecular dynamics (MD) simulations and finite element (FE) method based on the boundary layer model, respectively. The silicon-silicon (Si—Si) bond in the FE method is modeled as a nonlinear Timoshenko beam based on the Tersoff potential (T3) for the first time, where all the parameters of the nonlinear beam are completely determined based on the continuum modeling. The present MD and FE results show that both critical SIFs and crack growth angles obviously depend on chiral angles, thicknesses and loading angles of SCS plates. Our FE results agree well with those from present MD simulations using the modified Tersoff potential. Checking against the SIFs of available results shows that present MD and FE results are reasonable. This study should be of great help for understanding thickness- and chirality-dependent fracture properties of SCS and designing silicon-based nanodevices.

1. Introduction

SCS is a perfect crystal and possesses its unique mechanical and physical properties, which is widely used in integrated circuits, solar cells and micro-electromechanical systems (MEMS) industries [1–3]. With the development of industrial technology, more and more electronic components become smaller and thinner, even most of those components work under micro/nanoscale condition [4,5]. The sensing or actuating parts of MEMS consist of micro/nano-scaled structures, e.g., cantilevers, bridges and plates, which are usually made of silicon. The size- and chirality-dependent properties of these micro/nanostructures have to be tailored and the residual stresses after the fabrication have to be assessed to design MEMS with certain properties. In particular, it is necessary to understand fracture properties of SCS under complex loading conditions in order to design and assemble silicon-based nanodevices.

Great efforts have been made to identify the mechanical properties of silicon. Zhang et al. [6] detailedly explored the anisotropic elasticity of silicon by a matrix-based computer algorithm and also gave the relationship between the thermal deformation and the Poisson's ratio. Zhu et al. [7] reported the first atomistic determination of the minimum energy path for a series of bond ruptures to advance a crack front. Hauch et al. [8] measured the velocity of a running crack in brittle SCS as a function of energy flow to the crack tip, in which their experiments were validated by direct comparison with MD simulations based on the modified Stillinger-Weber (SW) interatomic potential. Buehler et al. [9,10] revealed that the crack speed of SCS should jump from 0 km/s to 2 km/s by

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employing a multiparadigm simulation of a hybrid ReaxFF-Tersoff model. At the same time, Cook [11] studied the strength and sharp contact fracture of silicon and found the fracture properties of silicon with different contact flaws. Bailey and Sethna [12] presented the fracture properties of SCS at atomically sharp notches with different opening angles using MD simulations, where the relationship between the critical SIFs and the opening angles was derived. Masaki et al. [13] investigated the effect of dopants and precipitations on the brittle-to-ductile transition in SCS. Masolin et al. [14] gathered the mechanical properties of SCS between 293 K and 1273 K and discussed their validity from previous literatures.

Despite the fact that the above mechanical properties of SCS were studied, the size- and chirality-dependent mixed-mode I-II fracture properties of SCS are not clear yet. In particular, the systematical study on their fracture properties using MD simulations based on the boundary layer model has not been reported till now. On the other hand, despite the importance of available MD simulations [8–10] and constitutive models [6], the link between molecular and continuum descriptions of the fracture properties is still not well established. To avoid the high computational cost of MD simulations and overcome limitations of continuum models, the FE method should be an effective way to study the fracture properties of SCS.

Due to the approximate isotropic material of SCS [15], it is suitable to use the traditional boundary layer approach to study their fracture properties.

In this paper, the thickness- and chirality-dependent mixed-mode I-II critical SIFs and crack growth angles of SCS [1 0 0] and [1 1 0] plates are studied using MD simulations and FE method based on the boundary layer model, respectively. The Si—Si bond in the FE method is modeled as a nonlinear Timoshenko beam based on the Tersoff potential (T3) for the first time, where all parameters of the nonlinear beam are obtained based on the continuum modeling. Due to the structural symmetry, the chiral crack angles of [1 0 0] plates ($\alpha = 0^\circ, 30^\circ, 60^\circ, 90^\circ, 120^\circ, 150^\circ$) and [1 1 0] plates ($\alpha = 0^\circ, 15^\circ, 45^\circ, 90^\circ, 180^\circ$ and 270°) with different thicknesses are studied under different loading angles from $0^\circ \le \varphi \le 90^\circ$ (Note that $\varphi = 90^\circ$ represents the pure mode I and $\varphi = 0^\circ$ is the pure mode II), respectively.

2. Models and methodology

2.1. Boundary layer model

Williams [16] proposed an asymptotic expansion of the displacement field near the crack tip in an isotropic linear elastic body. In a thin elastic disk, the three-dimensional (3D) stress concentration region is mainly within the distance of 1.5 times as far as the thickness (t) of the disk from the crack front, as shown in Fig. 1. However, the 3D character of the stress field is clearly observed in the region of around $0.5\,t$ [17,18]. That is to say, the outer boundary of the disk in Fig. 1 meets the plane stress state when $R_0/t > 1.5$ [17,18], where R_0 is the radius of the disk. Since the higher order term of the T-stress in the Williams' asymptotic solution is very small along the crack-tip region by comparison with the lower order singular term, the nodal (or atomic) displacements on the outer boundary of the disk regardless of T-stress term can be expressed as

$$u_x = \frac{1+v}{E}\sqrt{\frac{r}{2\pi}}\left[K_{\mathrm{I}}^{\mathrm{far}}\cos\frac{\theta}{2}\left(k-1+2\sin^2\frac{\theta}{2}\right)+K_{\mathrm{II}}^{\mathrm{far}}\sin\frac{\theta}{2}\left(k+1+2\cos^2\frac{\theta}{2}\right)\right] \tag{1}$$

$$u_y = \frac{1+v}{E}\sqrt{\frac{r}{2\pi}}\left[K_{\mathrm{I}}^{\mathrm{far}}\sin\frac{\theta}{2}\left(k+1-2\cos^2\frac{\theta}{2}\right)-K_{\mathrm{II}}^{\mathrm{far}}\cos\frac{\theta}{2}\left(k-1-2\sin^2\frac{\theta}{2}\right)\right] \tag{2}$$

where r and θ are the radius of the disk and the polar angle in Fig. 1, respectively. u_x and u_y represent the in-plane displacements along the x and y directions, respectively. E is the Young's modulus and v is the Poisson's ratio of the disk. Note that $v = 0.273$ is

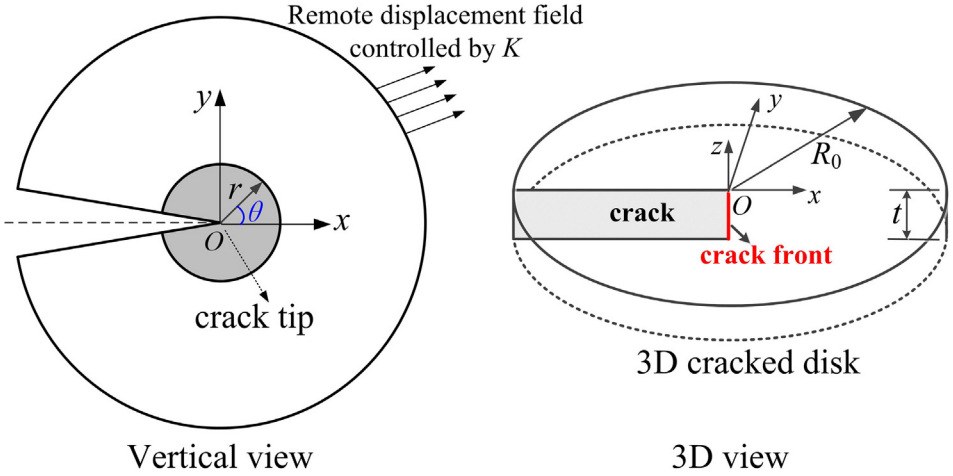

Fig. 1. Illustration of the problem and the coordinate system of a 3D cracked disk.