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Stress analysis in scratching of anisotropic single-crystal silicon carbide

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ABSTRACT

An expression for the stress distribution around an indenter in scratching of anisotropic single-crystal silicon carbide is derived by the superposition of the elastic stress field and residual stress field. It is an extension of isotropic materials. The elastic stress field can be obtained from the solutions of a point force problem in semi-infinite anisotropic materials using Green's function method. The calculation of residual field due to plastic deformation adopts a center of dilatation model. The plastic deformation zone beneath the indenter is simplified to a hemisphere based on the crystal-plasticity theory for single-crystal silicon carbide. The dilatation of the hemispherical plastic zone attached on the free surface of a semi-infinite solid is solved by a doublet force system. The values of stresses obtained from this calculation method match well with those calculated using classical solutions when the problem degenerates into isotropic materials. In addition, the stress field when scratching on the (0001) plane of 4H-SiC with a conical diamond indenter is presented using the new calculation method. In previous studies, the 4H-SiC was usually simplified as isotropic materials. However, it is found that the values of tensile stresses along the *c*-axis leading to median cracks are 1.4 times higher than those in isotropic materials. Therefore, it is not appropriate to simplify the single-crystal silicon carbide as an isotropic material when analyzing the scratching-induced stress field.

1. Introduction

Single-crystal silicon carbide (SiC) has been a promising material due to its excellent mechanical strength, good chemical resistance, and high thermal conductivity. Among these single-crystal SiC with approximately 250 polytypes, 4H-SiC and 6H-SiC are of particular interest and are considered to be a typical third generation semiconductor material in the micro-electronic field [1,2]. However, median cracks may generate on the subsurface layer of SiC wafers in the manufacturing process of wafers due to its high hardness and brittleness [3]. The cracks need to be removed as they can increase the breakage risk of wafers. Based on the fracture mechanism of brittle materials, the generation of median cracks is closely related to the stress field during the manufacturing process, and is influenced by the crystal structure of anisotropic materials [4]. Therefore, it is necessary to study the stress field in anisotropic single-crystal SiC in order to control the subsurface damage induced by median cracks.

The manufacturing process of single-crystal SiC, such as wire sawing and grinding, can be regarded as a complex scratching process by randomly distributed abrasives. The results of scratch or indentation tests have already been applied to the wire sawing and grinding process in order to deal with abrasive-workpiece interaction problems [5,6]. A theoretical contact model between the Berkovich indenter and work-piece in scratching of silicon carbide ceramics was established by Zhang et al. [7]. The apparent friction was divided into two components, the interfacial friction coefficient and the ploughing friction coefficient. Lawn and et al. [8] described the median crack system in ceramics by resolving the stress field beneath the indenter into the elastic stress component and residual stress component. Griffith fracture mechanics were employed to the approach to median cracks in their studies. Guo et al. [9] investigated the propagation of a subsurface-inclined crack in the scratching process of brittle crystal materials. The classical solutions of the scratching-induced stress field in isotropic materials were used to calculate stress intensity factors at the tip of cracks.

Researchers have focused on the stress field beneath the indenter in scratch or indentation tests in recent years. Zha et al. [10] obtained the stress distribution of a coating/substrate system after an indentation test using the finite element method. For the convenience of application, Yoffe [11] proposed an analytical stress model for the indentation on isotropic brittle materials by the superposition of the elastic stress and residual stress. The calculation of the elastic field adopted the Boussinesq solution for a point load in semi-infinite half-space, and the calculation of residual field adopted a center of dilatation model which can be equivalent to three doublet forces. The strength of the

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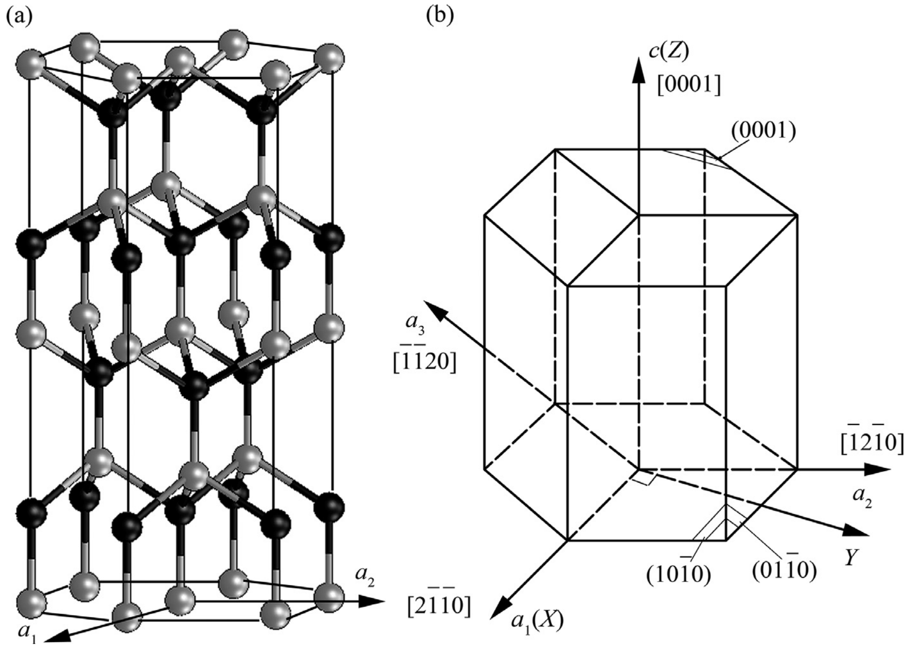

Fig. 1. The 3D crystal structure and coordinate systems of 4H-SiC.

residual field in Yoffe's model was analyzed by Jing et al. [12], which can be determined by the normal force, material properties and the indenter geometry. Fang and Zhang [13,14] applied the stress distribution to the investigation of the dislocation emission in silicon during indentation and nanoscratch, respectively. The research is based on the mechanism that with the increasing load, a phase transformation takes place in silicon before partial dislocation emission. Wang et al. [15] extended the indentation stress model into the scratching situation and calculated the stress field due to a tangential force applying the Cerruti solution. Feng et al. [16] showed the equivalence between an expanding cavity and a center of dilatation when calculating the residual field. Furthermore, an embedded center of dilatation model was proposed. However, the scratching-induced stress field still needs to be investigated for anisotropic single-crystal SiC as current works are mostly dealing with isotropic materials.

In this paper, the calculation model of the scratching-induced stress field is extended to anisotropic single-crystal SiC. The calculation method is given in Section 2. The elastic stress field due to a point force and the residual stress due to the plastic deformation zone are calculated considering the anisotropic structure. The verification of this method and the stress distribution when scratching on the (0001) plane are discussed in Section 3. We conclude with some remarks in Section 4. This paper will provide a better understanding of the stress field and the crack propagation in anisotropic materials.

2. Calculation of the stress field in single-crystal SiC

The stress field beneath the indenter in scratching of single-crystal SiC is calculated in this section. This calculation method is based on the anisotropic structure of single-crystal SiC. Therefore, the anisotropic crystal structure and anisotropic properties of single-crystal SiC should be discussed in advance.

2.1. Anisotropic properties of single-crystal SiC

4H-SiC and 6H-SiC both have the hexagonal crystal structure and P63mc symmetry, so that it is enough to discuss the case of 4H-SiC in this paper. The 3D crystal structure and coordinate systems of 4H-SiC are shown in Fig. 1. Orthogonal coordinate systems (X, Y, Z) are used to write out the compliance or stiffness matrices instead of crystal axes (a_1, a_2, c).

Table 1
Elastic constants of 4H-SiC and 6H-SiC [1,18].

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}
4H-SiC	507	108	52	547	159
6H-SiC	501	111	52	553	163

Young's modulus for an arbitrary plane in materials with hexagonal structures can be obtained from the following equation [17]:

$$E^{-1} = s_{11}\sin^4\psi + s_{33}\cos^4\psi + \left(s_{44} + 2s_{12}\right)\sin^2\psi\cos^2\psi \tag{1}$$

where ψ is the included angle between the c axis and the normal direction of the plane to be solved, s_{ij} is the compliance matrix which is the inverse of the stiffness matrix, the stiffness constants of 4H-SiC and 6H-SiC are shown in Table 1.

The Poisson's ratio for an arbitrary crystal plane can be expressed as [17]

$$\upsilon = -\frac{s_{12}\sin^2\psi + s_{13}\cos^2\psi}{s_{11}\sin^4\psi + s_{33}\cos^4\psi + \left(s_{44} + 2s_{12}\right)\sin^2\psi\cos^2\psi} \tag{2}$$

The scratching process is supposed to be carried out on the (0001) plane of single-crystal SiC as shown in Fig. 2, because the (0001) crystal wafer is mostly used in practical applications. The scratching direction is along the Y-axis. It should be noted that the scratching direction in the (0001) plane does not affect the stress field due to the isotropic properties of the (0001) plane which can be easily proved by Eq. (1).

A plastic deformation zone is found beneath the indenter, and the subsurface crack will propagate at the bottom of this zone as a result of the existing stress field. The stress field can be obtained by the superposition of the elastic stress field due to the scratch force and residual stress field due to the plastic deformation [11]. The two sources of the stress field are calculated in the following sections, respectively.

2.2. Elastic stress field

The elastic stress field due to the scratch force in scratching of single-crystal SiC is discussed in this section. The scratch force can be resolved