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Plastic Deformation and Residual Stresses in SiC Boules Grown by PVT

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Abstract

The thermoelastic stress distribution in growing 6H SiC crystals was simulated using a two dimensional finite element model. Based on the calculated stress distribution, possible plastic deformation of the material was postulated. High resolution x-ray diffraction (HRXRD) was used to detect the net deformation and residual stresses in the grown crystals. The results were in agreement with the postulated plastic deformation.

Introduction

One of the outstanding issues in SiC technology is the optimization of the bulk crystal growth process. Of particular interest is the relationship between growth conditions and the structural quality of boules. In recent years, several research groups have employed mathematical modeling to study this subject. Advanced models have been developed for simulating the global temperature distribution and growth rate by accounting for major features of the physical vapor transport (PVT) process such as heat generation by electromagnetic induction, heat transfer by conduction, convection, and radiation, mass transport, and chemical reactions [1-4].

Tsvetkov *et al.* [5] discussed the effect of thermal stress developed in growing or cooling crystals. They applied a one dimensional model in order to estimate the resolved shear stress in the basal plane glide systems due to an axial temperature gradient. They estimated that the stress in a 50 mm diameter crystal can be in the range of 0.1~100 GPa and concluded that this mechanism can be the main source of the basal plane dislocations.

In this study, we describe a two dimensional model of thermoelastic stresses in growing 6H SiC crystals which involves both an axial and a radial temperature distribution. The effect of stress distribution on the plastic deformation of SiC boules and the possible mechanisms of the deformation are considered.

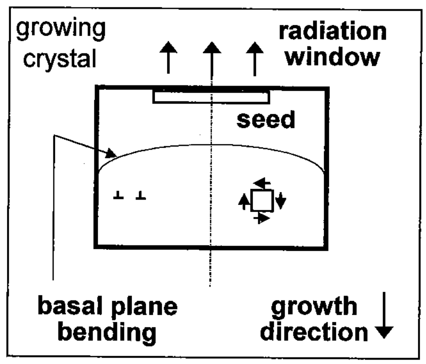

Fig. 1 Schematic showing the growth condition, the shear stress direction, edge dislocations involved, and the bending of the basal plane.

Finite Element Modeling

The distribution of various stress components was modeled using the ANSYS software package, employing the finite element method. The assumed growth conditions are illustrated schematically in Fig. 1. The cylindrical crystal grows downward. Heat is injected from the growth surface of the crystal (the bottom and lateral faces of the cylinder) and extracted through the radiation window at the top of the seed. Because of the geometry, an axisymmetric model along the growth direction (the [0001] direction) was used. With this assumption, the 3-D cylindrical problem can be simplified into a 2-D rectangular problem. Three normal and one shear component (σ_{rr}, $\sigma_{\theta\theta}$, σ_{zz}, σ_{rz}) out of the six independent 3-D stress components can be non-zero.

The growth surface of the crystal is allowed to move freely. The possible interaction between growing crystal and the crucible side wall was neglected for simplicity. Two opposite extreme boundary conditions were considered on the top face. It is set free to move in the first case and restricted not to bend vertically in the second case. These can be considered as conditions for two different seed mounting methods, simple mechanical and rigid glue mounting. In an actual growth with a glue mounted seed, the condition will not be as rigid as the second case and will be between the two extreme cases.

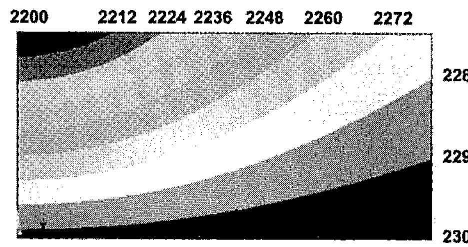

Fig. 2 A typical temperature profile in a growing crystal. (unit: °C)

One of the difficulties in the analysis is that the necessary material properties are not known at temperatures of the PVT growth process. Inoue and Kurachi [6] reported the anisotropic thermal expansion behavior of 6H single crystal from 850 °C to 2100 °C. We extrapolated their experimental data to the modeling temperature. The complete set of room temperature elastic constants was reported by Kamitani *et al.* [7]. Their temperature dependence was studied by Li and Bradt [8] and Samant *et al.* [9], but the highest temperatures used were only 1000 °C and 1300 °C, respectively. Thus, in this study, we applied the room temperature values for approximation.

Stress Distribution

In Fig. 2, a typical temperature distribution in a growing crystal is shown. The left side represents the center axis (the symmetry axis) and the right side is the crystal periphery. The diameter is 50 mm and the aspect ratio of crystal height to diameter is 0.25 in the case. Since the heat is extracted through a window over the center portion of the top face, the region is coldest during growth. In this particular case, the average axial temperature gradient along the symmetry axis is 80 °C/cm and the average radial temperature gradient at the top face 30 °C/cm. The cold temperature at the center of the top face is 2200 °C.

The resultant thermoelastic stress components due to temperature distribution of Fig. 2 are shown in Fig. 3, where (A~D) are for the case of mechanical mounting and (a~d) glue mounting method. The absolute maximum values of all the components are increased greatly when the displacement constraint due to glue mounting is considered. The distribution of each component is also influenced. This is especially true for the shear component, where a negative shear stress becomes dominant.

The normal stress components are tensional in the center of crystal and compressive in the outer edge as clearly shown in the case of mechanical mounting. The radial and tangential components are dominant. This can be expected since the center of crystal is cooler than the outer edge during growth. The effect is more pronounced in the region close to the top face where the radial temperature gradient is larger. For the glue mounting, the region where the compressive radial and tangential normal stresses are maximum moves from the outer edge to the center of the bottom face and the axial normal stress increases much more than the other components. These changes appear to be exaggerated and due to the simplified boundary conditions used. In an actual growth, as mentioned above, the glue mounting is not expected to be as firm as assumed by the model. The crystal periphery is also bounded by the crucible wall and can interact with it.

Crystal Response and HRXRD Measurements

The negative shear stress will cause the basal plane edge dislocations of the type shown in Fig. 1 to glide toward the center of crystal. The accumulation of such dislocations will cause the basal plane to bend to a shape as indicated, which is concave to the growth direction. The critical resolved shear stress for the glide system was reported to be 5 MPa at 1300 °C by Samant *et al.* [9]. The value is expected to be even smaller at the growth temperature. Thus, the magnitude of calculated shear stress appears to be large enough to activate the basal plane dislocation glide.

In addition to the shear component, crystal can deform in response to the normal stresses. From the distribution of normal stresses in Fig. 3, we suggest that the central region expands plastically during growth. If this plastic expansion occurs and relieves a certain amount of elastic stress at the growth temperature and if it isn't reversed and removed fully during cooling, the resultant plastic strain will be frozen into the boule after cooling and act as the source of residual stresses. The stress state after cooling will be opposite of that during growth, i.e. the periphery of crystal is expected to be under tension while the center be under compression. The plastic expansion is expected to occur by the slip of threading edge dislocations in the prism planes. The slip system $\langle 11\bar{2}0\rangle\{\bar{1}100\}$ has been reported active in PVT grown hexagonal SiC [10].

HRXRD mapping along diameters of the boules was used to capture the plastic deformation frozen in the crystals as well as the residual elastic strains. The crystals were sectioned horizontally in slabs thick enough to prevent bending due to residual stresses. The total orientation change of the basal plane along a boule diameter was typically in the range of 100~2000 arc seconds (Fig. 4). The shape of bending was consistent with the calculated shear stress direction as shown in Fig. 1. Continuous reduction of the c-lattice spacing was observed along the radii of crystals from the center to the edge, which is consistent with the expected residual normal stress that is tensional along the radial and tangential direction and compressive along the axial direction. The amount of strain at the edge compared to the center was typically (-0.006) ~ (-0.002) % (Fig. 5).

Acknowledgements

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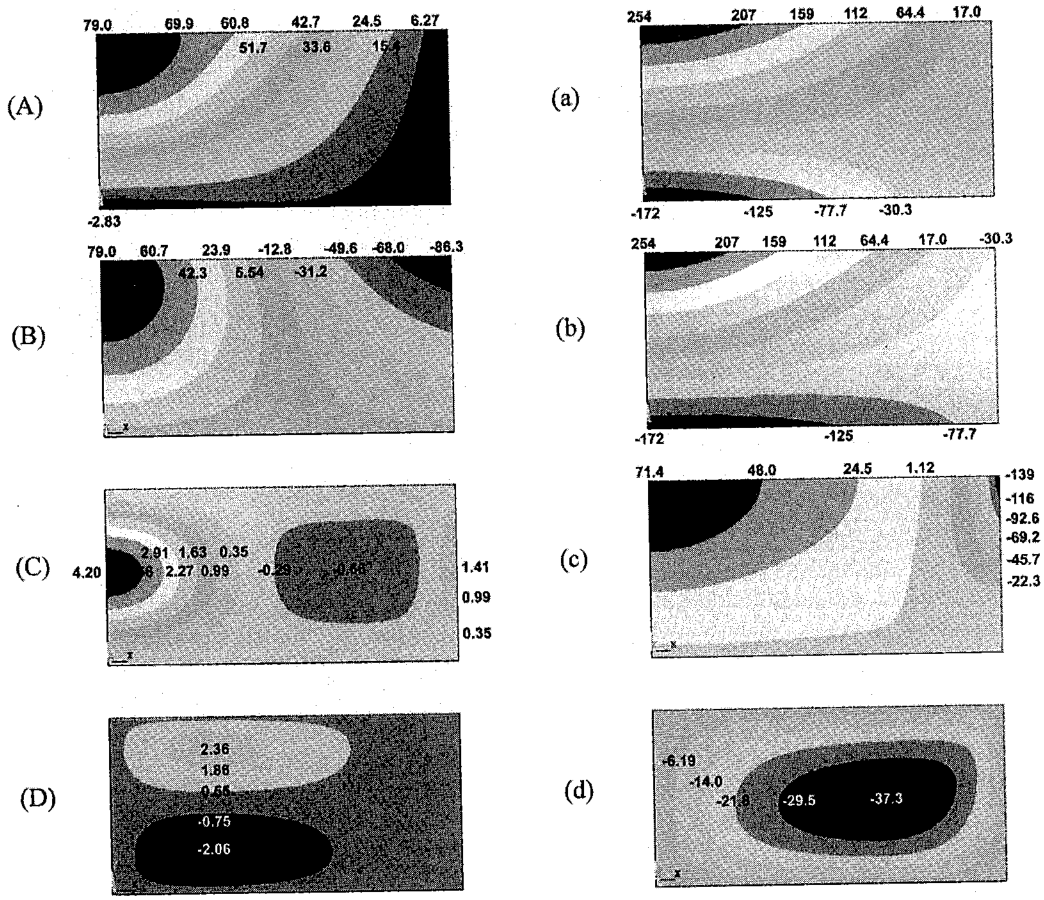

Fig. 3 Distribution of four non-zero stress components in the crystals during PVT growth for the two cases of mounting practice; (A~D) mechanical mounting, (a~d) glue mounting (unit: MPa)
(A, a) radial normal stress σ_{rr} (B, b) tangential normal stress $\sigma_{\theta\theta}$
(C, c) axial normal stress σ_{zz} (D, d) shear stress σ_{rz}

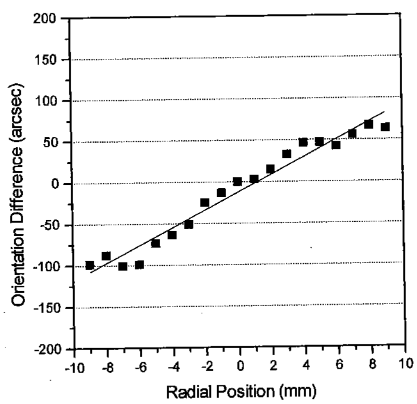

Fig. 4 Orientation difference of the basal plane along a crystal diameter with respect to the center position

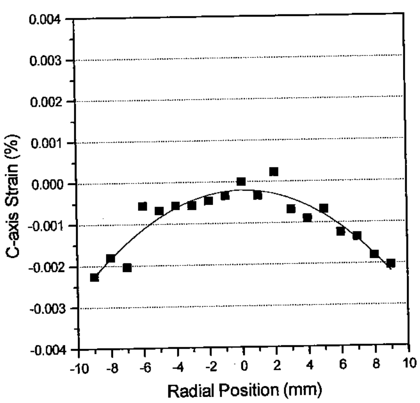

Fig. 5 The variation of strain of the c-lattice spacing along a crystal diameter due to the residual stress