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Extended Abstracts of the 2014 International Conference on Solid State Devices and Materials, Tsukuba, 2014, pp1000-1001

Structure of basal plane defects formed by the conversion of threading screw dislocation during solution growth of SiC

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1. Introduction

Silicon carbide (SiC) is a promising material for next-generation power device because of its excellent physical properties [1]. For the SiC power devices with high performance and long-term reliability, high-quality SiC wafers with low-dislocation density are necessary [2]. Solution growth method is one of the methods to produce high-quality SiC wafers [3-7]. Recently we have revealed that threading screw dislocations (TSDs) were converted to basal plane defects during the solution growth of 4H-SiC [5, 6]. The TSD conversion would produce high-quality SiC crystal because the converted defects laterally extend toward outsides of the crystal as the growth proceeds. Actually low-dislocation-density 4H-SiC crystal was achieved utilizing the TSD conversion [7]. In the present study, to reveal the mechanism of the TSD conversion, we investigated the structures of the basal plane defects formed by the TSD conversion.

2. Experimental

4H-SiC crystal was grown in a radio frequency-heated graphite hot-zone furnace (Nisshin-Giken Co., Ltd.) by top-seeded solution growth method. The solution was placed in a graphite crucible and kept in a vertical temperature gradient of 30 K/cm under a high-purity (>99.9999 vol.%) Ar gas flow. The graphite crucible had an inner diameter of 45 mm and was 50 mm high, and the graphite rod was 10 mm in diameter. 4H-SiC(0001) Si face crystals (10 mm × 10 mm) with 4° off-cut towards [$11\bar{2}0$] were used as the seed. The Si for the solvents had a purity of 11N (Tokuyama Co., Ltd.). Carbon was supplied from the graphite crucible. Prior to growth, the 4H–SiC seed crystal and the Si were cleaned by sonication in methanol, acetone, and purified water (18 MΩ·cm). The growth procedure was as follows: (1) the crucible was heated to 1973 K for 1.5 h; (2) the seed crystal, which was mounted on a graphite rod, was immersed in the solution and held there during the growth period; (3) the grown crystal was then removed from the solution. The crucible was rotated by applying the accelerated crucible rotation technique (ACRT). The crucible and the seed crystal were counter rotated with alternating rotation directions. The maximum crucible and seed rotation speeds were 20 rpm in each case. Residual solvent on the crystal was removed by etching in an HNO_3 + HF solution (HNO_3:HF = 2:1).

Position of the basal-plane defects were confirmed by X-ray topography and molten KOH etching. Grazing incidence synchrotron reflection X-ray topography measurements were performed at the high-resolution X-ray diffraction station BL15C in the Photon Factory at the High-Energy Accelerator Research Organization, Japan. The applied **g** vector was $11\bar{2}8$. X-ray topography images were captured on a nuclear emulsion plate (Ilford L4, 25 μm). KOH etching was carried out in a nickel crucible at 793 K for 3 min.

The structure of the basal-plane defects were investigated by transmission electron microscopy (TEM). The TEM specimens were fabricated by focus ion beam (FIB) method using FB-2100 (Hitachi Co. Ltd.). High resolution TEM observation was carried out by using JEM-1000K RS operated at 1000 kV.

3. Results and discussion

Figure 1 shows the X-ray topography image of the seed crystal and the grown crystal, and molten KOH etching surface of the grown crystal at the same position. In the image of the grown crystal, asymmetric knife-shape contrast of the basal plane defects extending to the step-flow direction were observed, instead of the circular contrast of TSDs. The basal plane defects were originated from the position of the TSDs in the seed crystal, which indicates that the TSDs were converted to the basal-plane defects during the solution growth as we have previously reported [5]. The basal plane defects were terminated at the surface where etch pits were formed. The shape of the etch pits for the basal plane defects were different from that of other

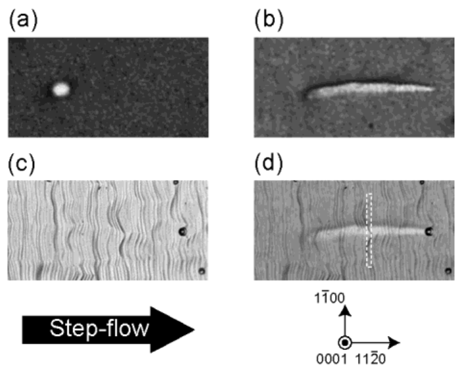

Figure 1: Synchrotron X-ray topography image (a) before and (b) after crystal growth. (c) KOH etching surface of the grown crystal. (d) Superposed image of (b) and (c).

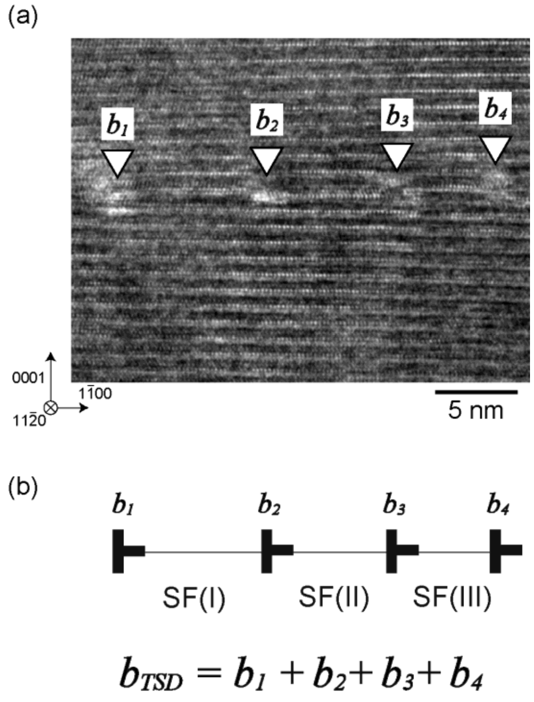

Figure 2: (a) Cross-sectional TEM image of the basal plane defect formed by the TSD conversion during the solution growth. (b) Schematic illustration of the core structure for the basal plane defect.

defects such as TSDs, threading edge dislocations (TEDs) and basal plane dislocations (BPDs). Thus, the position of the basal plane defects can be identified from the etching surface. TEM specimens were prepared by FIB at the position indicated by the dashed line in Fig. 1(d).

Figure 2 shows the cross-sectional TEM image of the core of the basal plane defect formed by the TSD conversion. The basal plane defect was extended dislocation composed of 4 Frank partials accommodating with stacking fault between them. Each partial dislocation corresponds to the insertion of one Si-C bi-layer and totally 4 bi-layers are inserted by this defect. This indicates that the Burgers vector was preserved after the TSD conversion. 4 partial dislocations were separated by the stacking faults of about 10 nm.

By the dissociation of partial dislocaitons, elastic strain energy of the dislocation is reduced. Figure 3 shows the elastic strain energy of dislocations with the Burgers vector of [0001] based on the anisotropic elasticity theory using the reported elastic constant of 4H-SiC [8, 9]. In the case of the perfect dislocation, TSD propagating to the [0001] direction is most stable and the basal plane defect is energitically unfavored. On the other hand, in the case that the dissociation of dislocation on the basal plane is taken into consideration, the basal plane extended dislocation is energitically as stable as the TSD. This indicates that the reduction of elastic strain energy by the dissociation of partial dislocations in the basal plane would be contributed to the TSD conversion phenomenon.

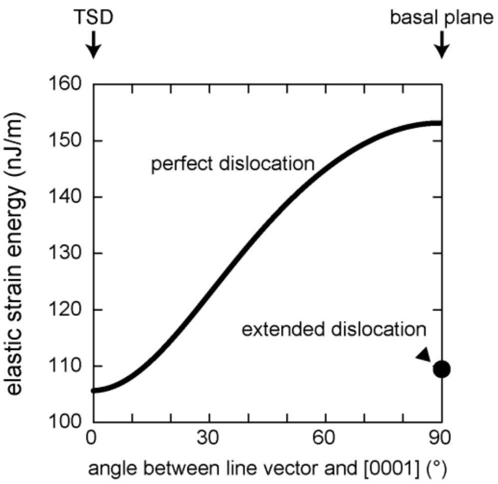

Figure 3: Orientation dependency of elastic strain energy for the dislocation with the Burgers vector of [0001]. In the case the dissociation of dislocations is taken into consideration, the elastic strain energy is largely reduced.

4. Conclusions

We investigated the structure of basal plane defects formed by the TSD conversion during the solution growth. The defects are extended dislocations composed of 4 partial dislocations accommodating with stacking fault between them. From the elastic strain energy calculation, extended dislocations on basal plane is as stable as TSD, which would be contributed to the TSD conversion phenomena

Acknowledgements

This study was partly supported by Grant-in-Aid for Scientific Research (23246004 and 24686078). The X-ray topography has been performed under the approval of the Photon factory program advisory committee (Proposal No. 2011G247).

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