Investigation of the step structure on the (0001) facet of physical vapor transport-grown 4H-SiC crystals on an off-axis seed crystal

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The surface morphology of the as-grown surface of SiC bulk crystals is crucial for polytype-preserving crystal growth of SiC by the physical vapor transport (PVT) growth method. The surface is covered with surface step trains advancing in the <1100> directions [1–4], and instabilities in these step trains, such as step bunching and/or meandering, would give rise to uncontrolled nucleation of foreign polytype crystals on the resulting wide (0001) terraces. The nucleation of foreign polytype crystals on the (0001) facet results in the formation of crystallographic defects in grown crystals and thus is one of the critical issues for the PVT growth technology of SiC crystals. PVT-grown 4H-SiC crystals are often grown on an off-axis (0001) seed crystal because of the improved production yield of off-axis substrates sliced from one single crystal boule used for subsequent homoepitaxial growth process. The off-axis (0001) seed crystal gives rise to the formation of the (0001) facet in an axially-asymmetric position on the growing crystal surface of a 4H-SiC boule. Such an asymmetric configuration of the (0001) facet on the growing crystal surface causes an asymmetric modulation in the step structure on the (0001) facet and could influence the polytype instability during PVT growth of SiC crystals; the facet surface regions located near the center and the periphery of the grown boule would show different step structures and thus result in different polytype instabilities.

This paper investigates the surface morphology on the (0001)C facet of a 4H-SiC boule grown on a 4° off-oriented (0001) seed crystal, focusing on the difference in the step structure on the facet edge regions located close to the center and the periphery of the grown boule. It was found that the axial-asymmetry of the facet location on the growing crystal surface of the boule caused different local inclinations of the as-grown surface at the facet edges close to the boule center and the periphery. We also found that the facet edge regions close to the center and the periphery of the grown boule showed fairly different step structures, in which a large non-uniformity of terrace widths between the surface steps was established on the facet edge region close to the boule center.

Two-inch diameter 4H-SiC single-crystal boules were grown on a 4° off-oriented (0001) 4H-SiC seed crystal by the PVT growth method. The typical growth temperature was approximately 2300–2400 °C, and the argon gas pressure was maintained between 1.0–2.0 kPa during growth. The grown boules were nitrogen-doped, and they contained nitrogen donors in the mid-10^{18} cm^{-3} range. Macroscopic (millimeter scale) morphology of the (0001)C facet of 4H-SiC boules was examined by differential interference contrast optical microscopy (DICM) and confocal laser scanning microscopy (CLM). The surface morphology assessments with micrometer- and nanometer-scale resolutions were performed by low-voltage scanning electron microscopy (LVSEM) and atomic force microscopy (AFM).

Figure 1(a) shows an AFM image of the step structure observed on a facet edge region close to the center of a PVT-grown 4H-SiC boule. As seen in the figure, the facet surface was covered with macrosteps of approximately 6–10 nm in height. A magnified AFM image of a terrace region between the macrosteps is shown in the inset of the figure, in which surface steps of 0.25 nm in height were clearly observed. They correspond to single SiC bilayer steps on the (0001) surface. It was found that the distance (terrace width) between single bilayer steps was not uniform, as shown in the magnified AFM image, and narrower and wider terraces were alternately arranged on the macrostep terraces; their widths are denoted as \( T_2 \) and \( T_4 \), respectively, as indicated in the magnified AFM image. We also observed surface steps of 0.5 nm in height on relatively narrow macrostep terraces; they would correspond to half-unit cell height steps having one or two dangling bonds per silicon atom at the step.
riser [5], and it was revealed that 0.25 nm height steps with a wider terrace width between them were formed as a consequence of decomposition of 0.5 nm height surface steps. We also conducted AFM observations of the facet edge region close to the boule periphery and found a similar step structure to that observed on the facet edge region close to the boule center, but a marked difference between the two regions exists in the degree of the non-uniformity of the terrace widths between 0.25 nm height steps. Here, we define the ratio of $T_1'/T_1$ as the degree of the non-uniformity of the terrace widths on the facet surface. Figures 1(b) and 1(c) show the occurrence frequency of the non-uniformity of the terrace widths between 0.25 nm height steps as a function of the $T_1'/T_1$ ratio on the facet edge regions close to (b) the boule center and (c) the periphery. As seen in the figures, the facet edge region close to the boule center exhibited a considerably larger non-uniformity of the terrace widths compared to the region close to the boule periphery.

At the conference, we will present more detailed information about the step structure on the facet edge regions and discuss the effect of the off-axis growth on the polytype instability during PVT-growth of 4H-SiC crystals.


Fig. 1. (a) AFM image of the step structure observed on a facet edge region close to the center of a PVT-grown 4H-SiC boule. The facet surface was covered with macrosteps of approximately 6–10 nm in height, and a magnified AFM image of a terrace region between the macrosteps is shown in the inset of the figure. (b) and (c) show the occurrence frequency of the non-uniformity of the terrace widths between 0.25 nm height steps on the facet edge regions close to the boule center and the periphery, respectively, as a function of the $T_1'/T_1$ ratio.