Dislocation Contrast Analysis on PVT-grown 4H-SiC through Synchrotron Grazing-incidence X-Ray Topographies and Ray-Tracing Simulation with Consideration of Surface Relaxation and X-Ray Absorption

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Silicon carbide (SiC) based power devices enable energy efficiency enhancement in power handling and conditioning owing to the combination of its superior electronic and physical properties, such as high thermal conductivity and high breakdown voltage. However, the degradation or premature breakdown of SiC power devices can be induced by crystallographic defects. Understanding the defect nature is therefore critical for improving growth strategies in order to control the defect density during crystal growth process. This study focuses on the investigation of dislocation configurations in physical vapor transport (PVT) grown off-axis 4H-SiC crystals. The image contrast of dislocations, such as basal plane dislocations (BPDs), deflected threading screw and mixed dislocations have been simulated through a sophisticated ray-tracing simulation model based on the principle of orientation contrast mechanism [1-7]. This simulation model is developed by considering both the effects of surface relaxation and X-ray absorption for evaluating the factors that contribute to the dislocation contrast formation. The simulated results are compared with the dislocation contrast images observed in synchrotron grazing-incidence X-ray topography. Analysis reveals surface relaxation effect as the dominate factor contributing to the dislocation contrast formation, which mainly occurs for diffractions near the crystal surface. Further investigation indicates that the diffracted X-ray beam from regions below the dislocation contribute additional contrast to the image. By taking X-ray absorption into account, the simulated dislocation contrast gradually weakens with a deeper diffraction position into the crystal. Based on the characteristic contrast of screw BPDs, Si-core and C-core edge BPDs, the full BPD loop contrast is also simulated. The Burgers vectors determination of all types of BPDs can subsequently be accomplished through comparison with the simulation.

Fig. 1. (a) Definition of a right-handed screw BPD in grazing-incidence X-ray topography. (b) Coordinate system used in the ray-tracing simulation.

Fig. 2. (a)(b) Simulated images of a right-handed screw BPD by stacking 10 μm layers from the crystal surface considering X-ray absorption (a) and considering both X-ray absorption and surface relaxation effect (b). (c) The actual grazing-incidence topograph from a 4° off-axis 4H-SiC wafer.