Dynamic behavior and atomic structure of twinning dislocations in sapphire

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Deformation twinning is one of the dominant plastic deformation modes in crystals. The propagation mechanisms of deformation twinning are typically explained by a shear process for each lattice layer, which is caused by twinning dislocations. For non-basal twinning in hexagonal crystals such as the {11-20} rhombohedral twinning is thought to be completed by not only simple shear but also atomic rearrangement (shuffling). This indicates that the motion of twinning dislocations in hexagonal crystal produces shear and shuffling. However, little is known about the dynamic behavior and the atomic structure of the twinning dislocations. In this study, we investigated the dynamic behavior and atomic structure of the twinning dislocations for rhombohedral twinning in sapphire (Φ#177;-Al_2O_3) by in situ transmission electron microscopy (TEM) nanoindentation and atomic-resolution scanning TEM (STEM).

A sapphire single crystal was cut to about 1.5 x 2.0 x 0.5 mm^3, and then the sample surfaces were polished to be a mirror finish. After the sample was mounted on a half-moon shaped mesh, it was thinned by mechanical grinding and Ar ion milling. In-situ nanoindentation experiments were performed using a TEM (JEM-2010HC, JEOL, 200kV) and a double-tilt nanoindentation sample holder (Nanofactory). The indentation direction was set to be [0001]. For atomic structure observations, the indented sample with twins induced by in situ TEM nanoindentation was further thinned by Ar ion milling. The twin/matrix interfaces were observed by annular bright-field (ABF) method using STEM (ARM-200F, 200kV, JEOL). Furthermore, the core structure of the twinning dislocation was examined by first-principles calculations using the VAPS program.

The formation of wedge shaped structures was observed by the indentation experiment. Electron diffraction analysis showed that the wedge shaped structures correspond to the {1-102}<-1101> rhombohedral twin. Twinning and detwinning phenomena were observed upon loading and unloading, suggesting that the rhombohedral twinning is reversible. ABF-STEM observations revealed that the twin/matrix interface has {1-102} terraces and ledges. The height of the ledges is equal to the spacing of {1-102} planes (= 3.48 Å). It can be said that this ledge structure corresponds to twinning dislocations. Thus, the motion of the ledges parallel to the {1-102} plane is related to twinning/detwinning, and the shuffling occurs within the range of 3.48 Å. An atomic structure model of the twinning dislocation was constructed based on our ABF-STEM observations, and the structure model was optimized by first-principles calculations. The optimized structure agrees well with the experimental images. In the presentation, we will show the dynamic motion and the core structure of the twinning dislocations, and discuss the twinning mechanisms based on our experimental and theoretical results.