Experimental and Theoretical Investigation of the Stacking Fault on the (0001) Plane in Alumina

Eita Tochigi¹, Teruyasu Mizoguchi², Atsutomo Nakamura³, Naoya Shibata¹, Yuichi Ikuhara¹,4,5

¹Institute of Engineering Innovation, The University of Tokyo, Tokyo, Japan.
²Institute of Industrial Science, The University of Tokyo, Tokyo, Japan.
³Department of Materials Science and Engineering, Nagoya University, Nagoya, Japan.
⁴Nanostructures Research Laboratory, Japan Fine Ceramics Center, Nagoya, Japan.
⁵Center for Elements Strategy Initiative for Structure Materials, Kyoto University, Kyoto, Japan.

Dislocations in alumina (α-Al₂O₃) have been studied for decades. The dislocations typically dissociate into some partial dislocations with a stacking fault, and the energetic stability of stacking faults is closely related to the dissociation reaction of a dislocation. So far, stacking faults on the {112₀}, {11₀₀} and (0001) planes have been extensively investigated [1-3]. However, there are a few experimental studies on the (0001) stacking fault. In this study, we investigated the atomic structure and the formation energy of the stacking fault on the (0001) plane formed between a dissociated dislocation in a low-angle grain boundary of alumina by scanning transmission electron microscopy (STEM) and theoretical calculations.

An alumina bicrystal with a (0001)/<11₀₀> 2° low-angle grain boundary was fabricated by joining a pair of single crystals at 1500°C in air. A TEM sample was prepared from the bicrystal by a standard technique including argon ion milling. The dislocation structure of the grain boundary was observed by annular bright field STEM (ARM-200F, 200kV, JEOL).

The (0001) stacking fault was examined by first-principles calculations using VASP code under the generalized gradient approximation. A supercell with 330 atoms was constructed on the basis of experimental observations. This supercell contains three equivalent stacking faults to satisfy the periodical boundary condition. A 4×1×2 k-point mesh was generated for Brillouin-zone integrations. The energy cutoff was set to be 500eV. Structure optimizations were performed to all the ions until the residual forces on the ions were less than 0.1 eV/Å under constant volume.

FIG. 1 shows an ABF-STEM image of a dislocation formed in the grain boundary viewed along the [11₀₀] direction. The dislocation is dissociated into two partial dislocations. They are separated on the (0001) plane, indicating the formation of a stacking fault on the (0001) plane. From the Burgers circuit in the figure, this dislocation has an edge component of 1/3[0001] in total. Since the 1/3[0001] vector does not correspond to a translation vector in alumina, this dislocation should have a screw component along the [1-100] direction. A more detailed analysis revealed that this dislocation has the Burgers vector of 1/3[1-1101] [4].

FIG. 2a shows an enlarged image of the (0001) stacking fault in FIG. 1. The stacking sequence of (0001) planes is found to be …1 2A 3 2B 1 2C 3 // 1A 2 1B 3 1C…, where ‘/’ indicates the position of stacking fault (Note that the stacking sequence of the perfect crystal is …1 2A 3 2B 1 2C 3 2A 1 2B 3 2C…, where 1 and 3 refer to the oxygen layer and 2A, 2B, and 2C refer to the aluminum layer.). This stacking fault is formed on the anion sublattice, although only the stacking faults on the cation sublattice have been reported in alumina. FIG. 2b shows a part of the atomic structure model with the (0001) stacking fault optimized by theoretical calculations. The configurations of ions in the experimental image and the theoretical model agree well with each other. The formation energy of the (0001) stacking fault was theoretically estimated to be 0.72 Jm⁻², which is about twice of that of the {112₀} and {11₀₀} stacking faults [3].

References:
Acknowledgement:

A part of this study was supported by the Elements Strategy Initiative for Structural Materials (ESISM) from the Ministry of Education, Culture, Sports, Science, and Technology in Japan (MEXT), and a Grant-in-Aid for Scientific Research on Innovative Areas “Nano Informatics” (Grant No. 25106003) from Japan Society for the Promotion of Science (JSPS), “Nanotechnology Platform” (Project No. 12024046) of MEXT, and JSPS KAKENHI (Grant Nos. 15H02290, 15H04145 and 15K20959).

FIG 1. ABF-STEM image of a dislocation having an edge component of 1/3[0001]. The dislocation is dissociated into two partial dislocations with a stacking fault on the (0001) plane. The positions of the partial dislocations are indicated by the arrows.

FIG 2. (a) Enlarged image of the (0001) stacking fault in FIG 1. (b) Atomic structure model of the (0001) stacking fault optimized by first-principles calculations.