TEM Study of Microstructure of MgO Σ5 (310)[001] Symmetrical Tilt Grain Boundary

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In electroceramic devices, electrical properties strongly depend on their grain boundary structures. It is known that unique electrical properties such as varistic effect often exhibit a grain orientation dependency due to a potential barrier enhanced by a local atomic structure. Especially, symmetrical tilt sigma (Σ) grain boundaries, which can be described by a mathematical 'coincidence site lattice (CSL) theory', tend not to show such electrical properties. On the other hand, a deviated boundary from exact Σ orientation relationship like a random grain boundary generates such electrical properties. As for the near-Σ boundary including a small deviation angle, it was reported that its misfit angle can be accommodated by periodically aligned (displacement shift complete) DSC dislocations and step structures. In order to understand such specific electronic transport mechanism, therefore, it is important to examine atomic structures in the near-Σ grain boundaries.

In this work, a magnesium oxide (MgO) was used as a simple model ceramic material and then examined two kinds of tilt near-Σ boundaries having deviation angles from exact Σ5 orientation relationship ($2\theta = 36.87°$) in MgO bicrystal*. These two specimens have small or large deviation angles of about 0.17° or 1.6° around [001] symmetric tilt axis. The MgO bicrystals were fabricated by annealing staked pairs of two single crystals at 1500°C for 10 hours in air. The specimens were thinned with conventional methods for a transmission electron microscopic (TEM) observation. TEM observations were performed by JEOL JEM-2010F (200 kV) or JEM-4010 (400 kV).

FIG. 1 is a dark-field (DF) image in the small deviated specimen which was taken under the condition that the boundary was largely inclined about 40° from an incoming electron beam direction. Dislocations exist periodically on the boundary. The dislocation intervals are about 40 nm or 5 nm depending on the deviation angles of 0.17° or 1.6°, respectively. HRTEM image for the small deviated specimen in FIG. 2 shows perfect joining at an atomic scale and no secondary phases. From the lattice fringes and the diffraction patterns, the actual tilt angles can be confirmed to be identical to the designed deviation angles.

If these dislocation are DSC dislocation, the dislocation intervals should be about 40 nm or 5 nm, to accommodate the deviated misalignment angles of 0.17° or 1.6°, respectively, based on the CSL/DSC theory in FIG. 3. Usually, a lattice displacement involving in a step structure should take place due to an introduction of DSC dislocations. However, such step structure could not be observed in these boundaries. The details will be reported.

*Z. Wang, M. Saito, K. P. McKenna, L. Gu, S. Tsukimoto, A. L. Shluger, and Y. Ikuhara, *Nature*, **479**, (2011) 380-383.

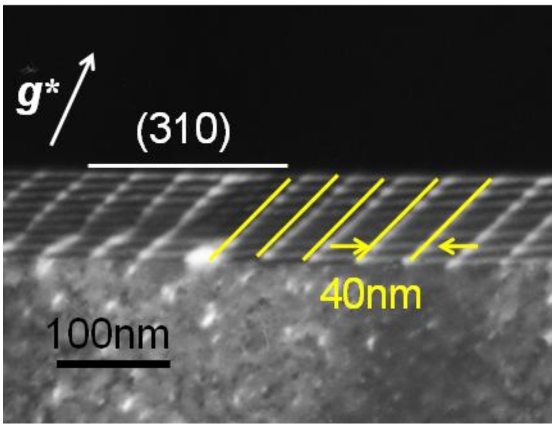

FIG. 1 Dark-field TEM image of MgO bicrystal Σ5 boundary.

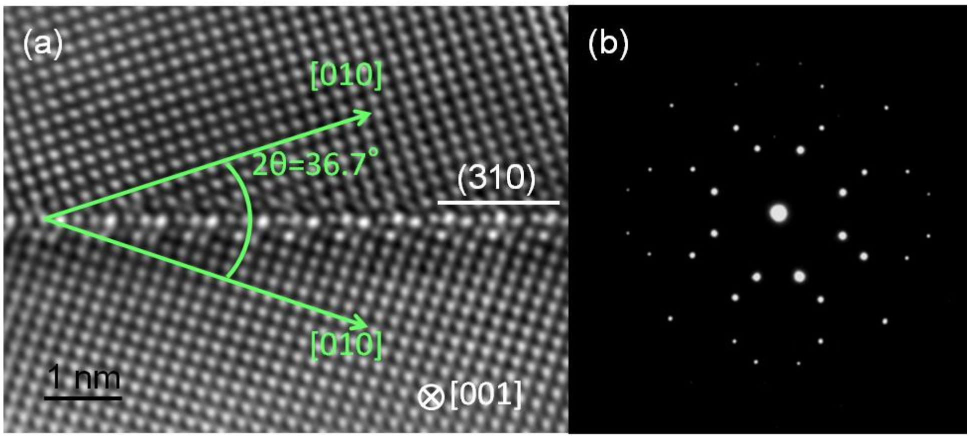

FIG. 2 (a) High-resolution TEM image and (b) selected area diffraction pattern of MgO bicrystal Σ5 boundary.

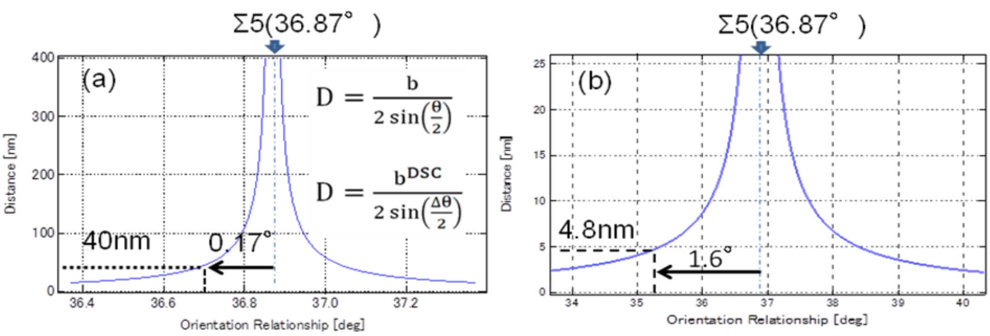

FIG. 3 The DSC plots indicate geometrically expected DSC dislocation interval for misorientation relationships of (a) 0.17°and (b) 1.6°.