Real materials including ceramics and minerals are, in general, of polycrystalline nature, and the prevailing presence of internal interfaces between grains, i.e., grain boundaries (GBs) often influences significantly their mechanical, electrical and physical properties. Magnesium oxide (MgO) is one of the best characterized oxide materials in terms of GBs and defects, and is often considered as a model oxide system owing to its simple rocksalt structure (with both the Mg and O atoms octahedrally coordinated) [1-2].

In this work, we investigated the microstructures of "near-Σ5" GB (Σ indicates the degree of geometrical coincidence at a GB ) in MgO in order to understand how the misalignment of tilting angles from the exact Σ5 orientation can modify GB structures at the atomic scale. Also it remains unknown whether impurities are segregated to the near-Σ5 GB and how such segregation can drive GB structure change and thus modify material property.

Here, we apply a bicrystal technique to fabricate a symmetrical tilt near-Σ5 GB with a bonding-angle deviation of ~1.7±0.1° from the exact Σ5 orientation, i.e., from the (310) plane. (S)TEM observations were performed by JEOL JEM-2010F (200 kV) and JEM-2100F (with Cs-corrector, 200 kV). Finally, we interpreted the GB local structure via mathematical approach based on O-lattice theory [3].

As a result, dark-field (DF) images showed periodically aligned edge dislocations on the boundary in order to compensate lattice mismatch due to misalignment. Annular bright field (ABF) images also revealed that the near-Σ5 GB comprises an alternating array of six normal Σ5 GB structural units and one deformed Σ17 GB structural unit, and importantly the Ca and Ti impurities are selectively segregated to the Σ5 units, while they are absent at the Σ17 units [4]. This near-Σ5 GB with tilting angle of 35.3° is mathematically equivalent to Σ33 GB on (227 0) plane. According to dissociation rule expected by O-lattice theory, this kind of GB with high Σ value can easily dissociate into two low Σ GB with special structure units, i.e., six Σ5 GB units and one Σ17 GB unit. This mathematical expectation is completely same as the obtained experimental result. The detailed will be reported.


Acknowledgement: This work was conducted in part at the Research Hub for the Advanced Nano Characterization and the “Nanotechnology Platform” at the Univ. of Tokyo supported by the MEXT of Japan and also at the Grant-in-Aid for Scientific Research (C) (grant no. 23560817) and the IKETANI and IZUMI Science Foundation for financial supports.