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Structural Transition of [001] Symmetric Tilt Grain Boundaries in Nb-Doped $SrTiO_3$

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It is well known that the grain boundary (GB) structure is closely related with the behavior of microstructural development as well as the resultant physical property. With this reason, a lot of studies have been theoretically and experimentally conducted to characterize the GB structure and GB energy in the various materials system, and thus diverse models, such as dislocation model, O-lattice model, coincident site lattice (CSL) model and displacement shift complete (DSC) model, have been proposed to explain the grain boundary structure. Especially when the symmetrically-tilted GBs have a small angle of tilt, within 15 degrees, and thus the dislocation cores do not overlapped, the classical dislocation model is most applicable to visualize GB as shown in the following equation [1,2].

$$\gamma_{gb} = \frac{\mu b \theta}{4\pi(1-\nu)}\left(1 - \ln\theta + \ln\frac{b}{2\pi r_0}\right),$$

where μ is the shear modulus, b is the Burgers vector, θ is the tilt angle, ν is the Poisson's ratio and r_0 is the dislocation core energy. This equation indicates that the GB energy increases in proportion to a tilt angle because the strain field along GB and density of dislocation are augmented.

So far, however, no atomic scale research on what is actually happening to the GB and dislocation cores along GB by increasing a tilt angle has been tried. To this end, we chose $SrTiO_3$ as a model system and a series of symmetric tilt bicrystals of Nb-doped $SrTiO_3$, from 4° to 18°, was prepared by joining two single crystals at 1873 K. The fabricated bicrystals were analyzed by high resolution transmission electron microscopy (HRTEM), high angular annular dark field-scanning transmission electron microscopy (HAADF-STEM) and electron energy loss spectroscopy (EELS). The 4°, 6°, 8° and 10°-tilted boundaries exhibit the array of the isolated dislocations cores but the dislocation core structure is changed from an in-line array of dislocation cores with Sr-excess and Ti-excess column core structures (fig. 1(a)) to a zigzagged array with only Ti-excess column cores (fig. 1(b)) as a tilt angle increases. By increasing a tilt angle further up to 18°, it is observed that the grain boundary structure changes from discrete configuration to a random configuration. More interestingly, two kinds of boundary region exist at the same boundary in case of the 14^o-tilted boundary as shown in fig. 2: one region with dislocation cores as found in 4°~10°-tilted boundaries and the other region with randomly oriented boundary as found in 18°. These structural changes are considered to be correlated with a minimization of strain energy due to elastic distortion between dislocation cores.

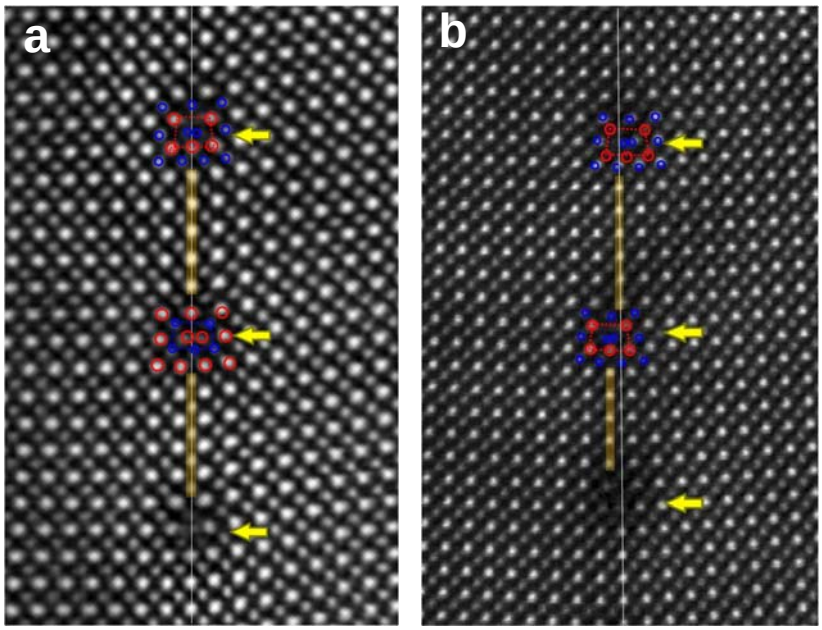

FIG. 1. HAADF-STEM images of (a) 6°-tilted GB and (b) 8°-tilted GB. The red and blue circles indicate Sr-Sr atomic column and Ti-O atomic column, respectively.

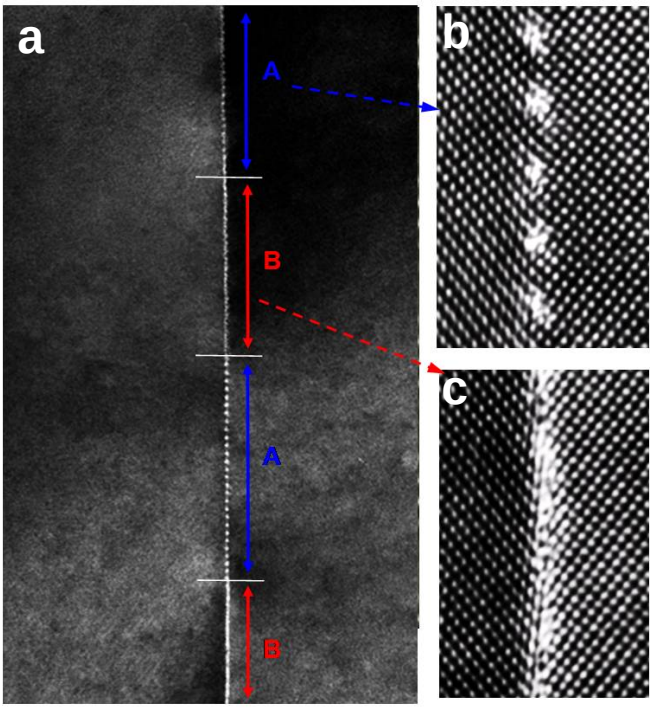

FIG. 2. (a) HRTEM image of 14°-tilted GB which consists of dislocation core region (A) and randomly oriented GB region (B). (b) and (c) are the enlarged HRTEM images of 'A' and 'B' in (a).

References

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2. W. T. Read and W. Shockley, Phys. Rev., 78, pp. 275 (1950).