Dislocation structure of low angle tilt grain boundaries in $LiNbO_3$

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$LiNbO_3$ is a widely used ferroelectric material with pyroelectric, piezoelectric, electro-optic and photoelastic properties, and a high Curie point (~1200 °C). Much research on $LiNbO_3$ has been conducted over several decades, most of which aimed at developing applications in optoelectronics, nonlinear optics, and electromechanical devices. However, it seems that basic topics such as the structure and behavior of lattice defects have not been studied adequately. In particular, the microscopic structure of plane and line defects in $LiNbO_3$ has received little attention, although the point defects have received attention because of their nonstoichiometry due to complex oxides.

Methods for $LiNbO_3$ crystal growth that decrease the plane and line defects and improve its optical performance have been studied. Deformation behaviors of $LiNbO_3$ have also been investigated from the viewpoint of the motion of the defects. For instance, Vere [1] and Blistanov et al. [2] investigated deformation twinning, while Fries and Péter [3] reported stress–strain curves and activated slip systems of single crystals. However, there is less knowledge about the microscopic structures of plane and line defects in $LiNbO_3$, because they have not been investigated using transmission electron microscopy and accordingly have not been identified at the atomic scale.

In this study, we investigate the structure of low-angle tilt grain boundaries in $LiNbO_3$ bicrystals, which was fabricated by the diffusion bonding of two single crystals, and characterize the microscopic structure of resultant boundary dislocations. The bicrystal experiment is powerful for characterizing the dislocation structure because an ideal array of dislocations is formed on the boundary [4].

A congruent $LiNbO_3$ single crystal grown by the Czochralski method was used to fabricate a bicrystal with a low-angle tilt grain boundary. The surfaces of the single-crystal plates were successively polished using diamond suspensions to achieve a mirror finish. The two single-crystal plates were subsequently joined by diffusion bonding in air at 800 °C for 10 h under an additional pressure of 0.1 MPa. Figure 1 shows an optical micrograph of the fabricated bicrystal. In the bicrystal, edge-type dislocations will be theoretically formed at the boundary.

Figure 2 shows a TEM image of the boundary dislocation array taken along $[10\bar{1}0]$ from a $\{\bar{1}2\bar{1}0\}$ / $<10\bar{1}0>$ low-angle tilt grain boundary. This image was taken using a high-resolution TEM (HRTEM) technique, although the magnification was not very high. The white arrows in the figure indicate the position of the boundary dislocations. The periodic spacing between two neighbor dislocations was about 27 nm.

Figure 3 shows a typical HRTEM image of the boundary dislocation, which directly includes one of the boundary dislocations. It should be noted that two neighbor lattice discontinuities clearly appear on the magnified HRTEM image. It can be seen that the two lattice discontinuities are the two dislocations with an edge component of $1/6[\bar{1}2\bar{1}0]$. It was found that the separation distance between the two dislocations was 2.7 nm along [0001], while the two are adjacently located along $[\bar{1}2\bar{1}0]$. It can be said

from direct observation by HRTEM that a boundary dislocation of $\boldsymbol{b} = 1/3[\bar{1}2\bar{1}0]$ dissociates into two partial dislocations with an edge component of $1/6[\bar{1}2\bar{1}0]$ by the narrow separation distance along [0001].

Thus, we succeeded in analyzing the structure of a boundary dislocation in $LiNbO_3$. It is interesting that the structure of a dislocation in $LiNbO_3$ seems to be similar to that of α-Al_2O_3 [5].

References

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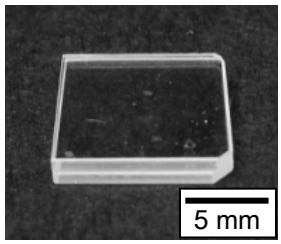

FIG. 1. Optical micrograph of the fabricated $LiNbO_3$ bicrystal.

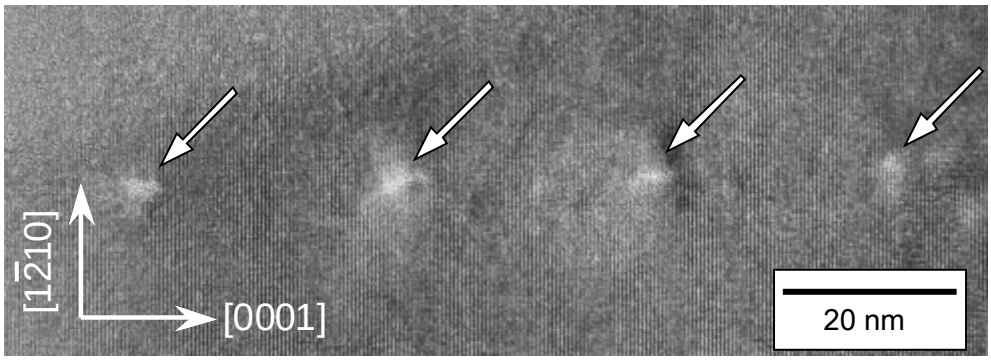

FIG. 2. Boundary dislocation array at a $\{\bar{1}2\bar{1}0\}$ / $<10\bar{1}0>$ low-angle tilt grain boundary

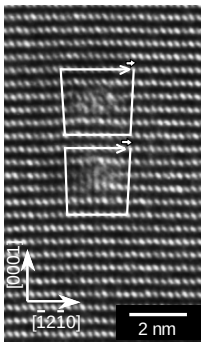

FIG. 3. A HRTEM image of a basal dislocation formed at the boundary in a $LiNbO_3$ bicrystal.