

TWIN BOUNDARIES IN LaNbO_4

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INTRODUCTION

The development of commercially viable solid-oxide fuel cells (SOFCs) presents great challenges in regard to materials selection and preparation. The need for long-term stability at elevated temperatures and for high electrical/ionic conductivity limits the possible materials for use as electrodes and electrolyte. LaNbO_4 is a material with potential use as an electrolyte or electrocatalyst in SOFCs, the present study investigates twinning in this system.

LaNbO_4 has a tetragonal high-temperature phase with space group $I4_1/a$ which transforms to a monoclinic low-temperature phase at roughly 500 °C. The low-temperature phase has space group $I2/a$ ($C2/c$) with a monoclinic angle $\beta=94.1^\circ$. Using the notation of Aizu (1) this is a ferroelastic transformation of the $4/mF2/m$ species, which produces twin domains in the plane containing the monoclinic angle. Sapriel (2) has predicted the domain-wall orientation for the ferroelastic species, and a calculation specifically for the LaNbO_4 system has been made by Jian and Wayman (3). These calculations predict that the domain boundaries should have an orientation parallel to the $(2\ 0\ -4.04)_I/(4.04\ 0\ 2)_{II}$ planes of the two domains. Evidence of this orientation has been observed, and based on HREM studies Jian and Wayman (3) have suggested a diffuse transition zone of about 25 Å between the twin domains.

RESULTS AND CONCLUSION

Nominally 5% Sr-substituted LaNbO_4 crystals were obtained by induction melting in a cold crucible. Most of the Sr appeared to have precipitated to a separate phase. The samples were ground in acetone and placed on a copper mesh. They were then studied in a JEOL 2010F electron microscope using selected area diffraction (SAD) and high-resolution electron microscopy (HREM).

SAD studies of the twins in the [010] projection reveal a splitting of reflections indicating that the domain lattices are related by a rotation of approximately β about the [010] axis, see Fig. 1a and 1b. These SAD patterns also suggest that the orientation of the domain boundary lies between the $(2\ 0\ -4)_I/(4\ 0\ 2)_{II}$ and $(2\ 0\ -6)_I/(6\ 0\ 2)_{II}$ planes of the two domains.

HREM studies along the [010] axis allow us to directly observe the domain boundary locally, see Fig. 1c and 2a. We observe that the change of contrast at the twin boundary reported by Jian and Wayman disappears when the electron beam enters the sample parallel to the boundary. Thus, there appears to be no disorder at the boundary, except possibly a slight bending of the lattice planes over a short distance. This direct observation of the twin boundary also allows us to determine the approximate orientation of the boundary. A model for the boundary based on the HREM image is presented in Fig. 2b. This model suggests a boundary parallel to the $\{2\ 0\ -6\}_I/\{6\ 0\ 2\}_{II}$ planes, which is in agreement with the SAD images obtained.

REFERENCES

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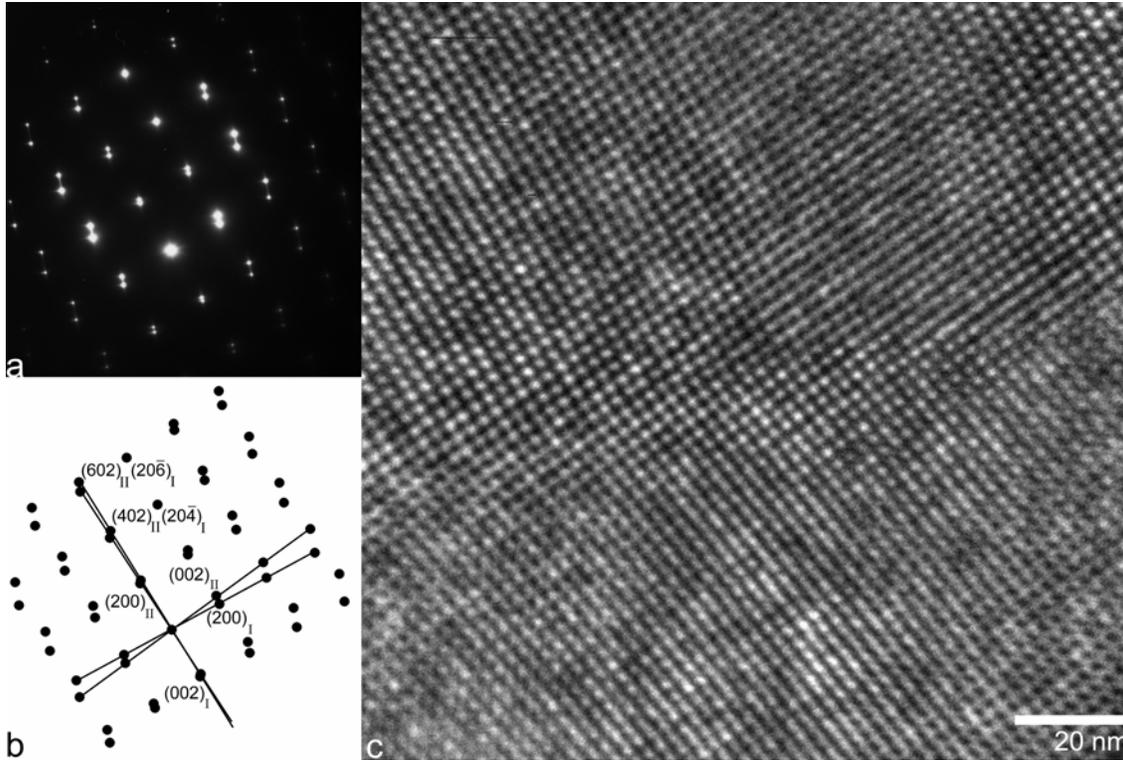


Fig. 1. a: SAD pattern from a twin boundary, notice the overlapping diffraction spots indicating parallel planes. b: The index of the SAD pattern in a. c: HREM image of a twin boundary.

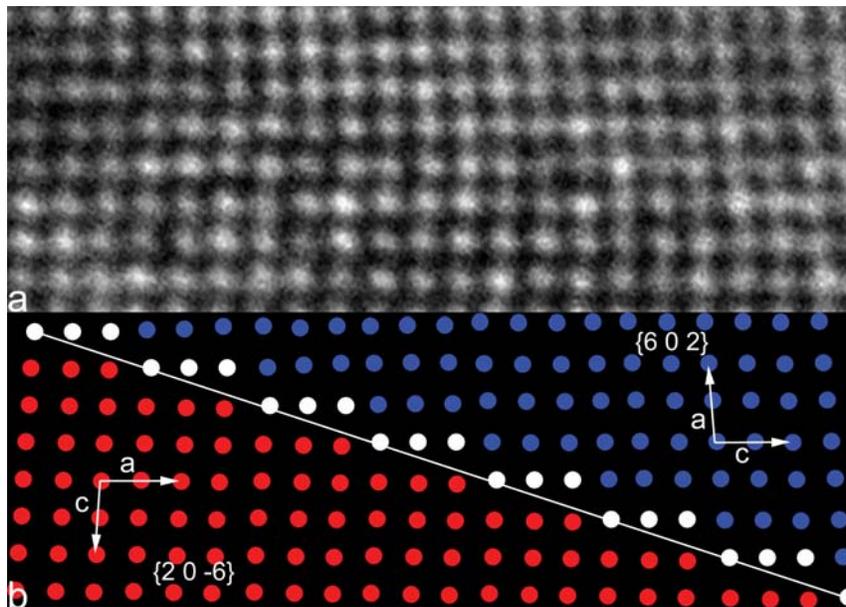


Fig. 2. a: Closeup of the twin boundary in figure 1c. b: Model of the boundary. The white dots indicate columns that are mutual to the two domains. The white line indicates the domain boundary.