DOI: 10.1017/S1431927605506469
Microsc Microanal 11(Suppl 2), 2005

Characterization of $Bi_{1.5}ZnNb_{1.5}O_{7-x}$ pyrochlore thin films by high-angle annular dark-field imaging in STEM

Dmitri O. Klenov, Jiwei Lu, Steffen Schmidt and Susanne Stemmer

Materials Department, University of California, Santa Barbara, CA 93106-5050

$Bi_{1.5}ZnNb_{1.5}O_7$ (BZN) is of interest because of its high dielectric constant, relatively low dielectric losses and high tunability [1]. However, its crystal structure is still not well understood. X-ray and neutron diffraction studies of the bulk material [2] showed that BZN had the cubic pyrochlore structure ($A_2B_2O_6O'$) with Bi and Nb occupying A and B sites respectively. The relatively small Zn cations, however, were found to occupy not only the B, but also the A sites, which is unusual [2]. Additionally, random displacements of the A-site cations from their positons in the ideal pyrochlore along six <112> were reported. The randomness of the structure is related to the dielectric properties of the material. Our recent dielectric measurements showed that BZN thin films show much improved loss properties at microwave compared to bulk ceramics of nominally the same composition [3]. Preliminary X-ray structure refinements were not sensitive enough to show differences between bulk and thin film structure. Moreover, X-ray diffraction only provides the average structure of the film and is not sensitive to local variations that may influence the dielectric properties. In this work we applied high-angle annular dark field imaging in scanning transmission electron microscopy (HAADF-STEM) characterize the structure of the films.

Conventional TEM showed that films are polycrystalline and free of extended defects. Figure 1 shows HAADF-STEM images taken along [110] and [112], respectively. The A and B sites can be clearly distinguished due to the differences in intensities, as expected from the Z-number sensitivity of these images. However, column intensities were not always consistent with expected cation occupancies from X-ray diffraction. Image simulations were used to distinguish between effects from sample thickness (column cross talk) and local ordering of cations.

A novel type of planar defect was also observed by HAADF-STEM (Fig 2). These defects were not visible in conventional high-resolution transmission electron microscopy. The intensity change at the defect plane was consistent with a complete site occupancy by bismuth. These planar defects were also observed along [112], which showed that they are parallel to the (111). The atomic structure of these defects and reasons for their formation will be discussed.

REFERENCES

[1] J. W. Lu, S. Stemmer, Applied Physics Letters **83**, 2411-2413 (2003).
[3] I. Levin, T.G. Amos, J.C. Nino, T.A. Vanderah, C.A. Randall and M.T. Lanagan, J. Solid State Chem., 168 (2002) 69.
[3] J. Park, J.W. Lu, S. Stemmer, R.A. York, J. Appl. Phys. (April 1, 2005 issue)

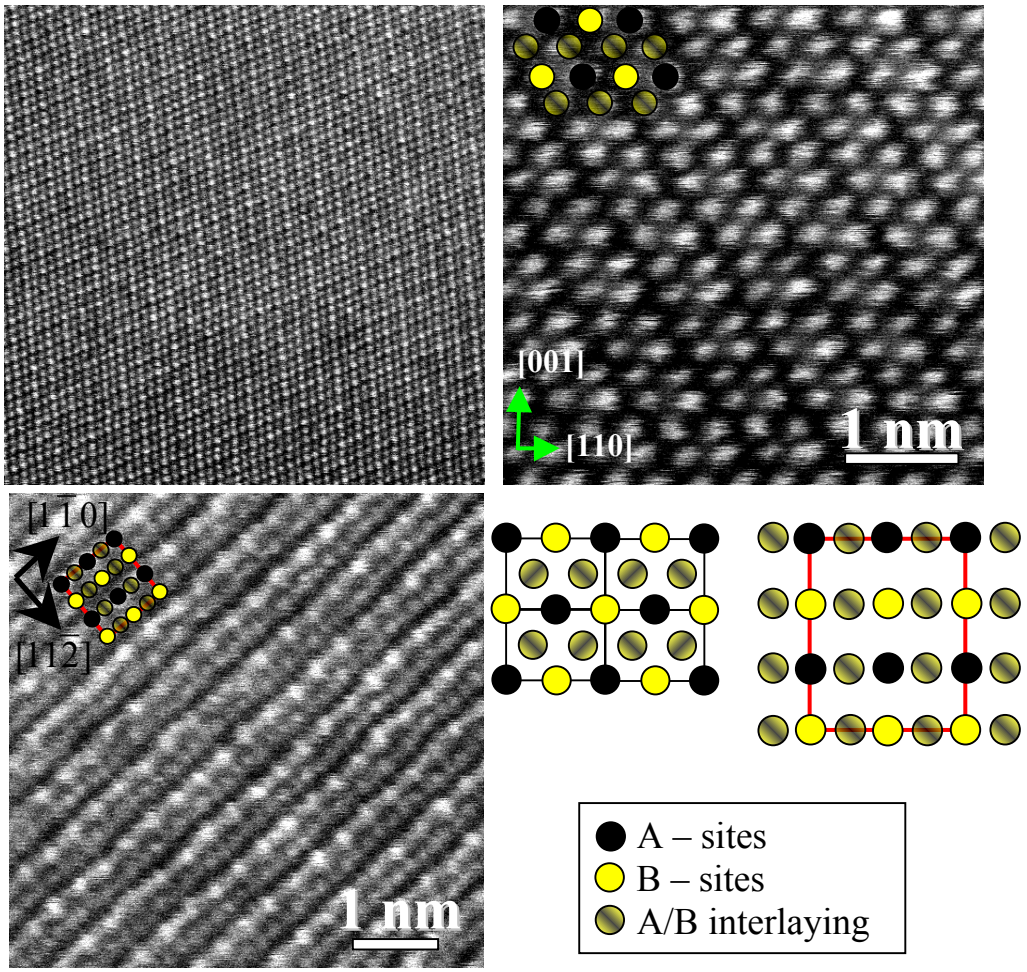

Fig. 1. HAADF-STEM images of the BZN film in [110] and [112] directions showing A and B sites of pyrochlore structure.

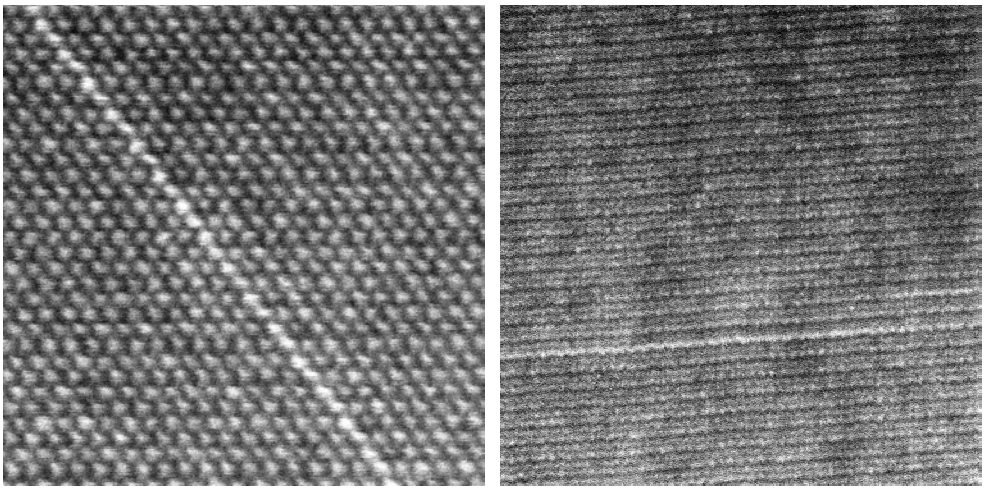

Fig. 2. HAADF-STEM images of the planar defect taken along [110] and [112] directions.

https://doi.org/10.1017/S1431927605506469 Published online by Cambridge University Press