

**MS13-1-10 Structure of Tetragonal Tungsten Bronze Materials by X-ray Diffraction and Electron Techniques**  
**#MS13-1-10**

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**Abstract**

Doped tetragonal tungsten bronze (TTB) materials based upon the filling of niobium-IV oxide sublattices with alkali and alkaline earth metals are receiving increasing interest for their ferroelectric and ferrorelaxor properties. Key to the development of improved materials is a firm understanding of the structure-property relationships, yet in many cases the results of structural assessments prove controversial. Of note for the present report is that of Sr<sub>2</sub>NaNb<sub>5</sub>O<sub>15</sub> (SNN) which is reported in the literature (García-González *et al.*, 2007) as crystallising with space group *Im2a* in cell setting [2 -2 0][2 2 0][0 0 2] with respect to the *P4mbm* aristotype. However, this is clearly at odds with the understanding of *c*-axis polarisation in these materials (Olsen *et al.*, 2016), and a recent group theoretical study (Whittle *et al.*, 2021) suggests a structure in space group *Ama2* and the supercell [1 -1 0][2 2 0][0 0 2] be most probable. We employ X-ray diffraction and electron techniques (Figure 1) to experimentally identify the principal structure of SNN and related materials, identifying an incommensurate phase that approximates the theoretically deduced *Ama2* structure.

Figure 1. (a) Dark field image and (b,c) selected area diffraction patterns of different twin domains at the indicated areas of a crystallite of SNN oriented along [1 1 0]. Imaging in (a) employs a diffracted beam at  $l=0.5$  where arrows in (b) and (c) show reciprocal lattice vectors with respect to the aristotype cell. Note the differing systematic absences between (b) and (c), apparent in the zero (ZOLZ) and first-order (FOLZ) Laue zones.

**References**

García-González, E., Torres-Pardo, A., Jiménez, R. & González-Calbert, J. M. *Chem. Mater.* (2007) 19, 3575-3580.  
 Olsen, G. H., Aschauer, U., Spaldin, N. A., Selbach, S. M. & Grande, T. *Phys. Rev. B* (2016), 93, 18010(R).  
 Whittle, T. A., Howard, C. J. & Schmid, S. *Acta Cryst.* (2021) B77, 981-985.

Figure 1.

