Investigation of Cation Ordering and Electronic Structures of $Ba_3BNb_2O_9$ (B = Co, Mn and Ni) Perovskites by Scanning Transmission Electron Microscopy

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One family of the complex perovskite $Ba_3BNb_2O_9$ (B = Co, Mn and Ni) has shown various properties both fundamentally interesting and technologically important. These oxides can be synthesized with ordered and disordered B sites, and the cation ordering of these compounds have effects on their physical properties. Advanced STEM techniques with sub-ängström resolution are provide powerful methods to investigate the B site cation ordering and electronic structures of these compounds.

Atomic resolution scanning transmission electron microscopy (STEM) high angle annular dark field (HAADF) imaging, or Z-contrast imaging allows us to directly image the cation ordering of these compounds, due to the large difference in the atomic number between B (Co, Mn and Ni) and Nb. The STEM HAADF Z-contrast image (a) next to the corresponding STEM ABF image (b) are shown in the **Figure**. The sketch in the figure depicts the projected atomic structure of the $Ba_3MnNb_2O_9$ along the [100] direction. In this projection, the Nb-Mn atomic planes are sandwiched between the Ba atomic planes, and the pure oxygen atom columns are between Nb and Mn columns. The Z-contrast image shows distinctly the much brighter Ba atom columns and the intensity alternating Mn and Nb columns (b). An intensity profile of this atomic plane (d) confirms very clearly the …Nb-Nb-Mn… ordering. Comparing to the Z-contrast image (a), (b) shows the exact the same scanning region of the STEM ABF image with the atoms now having a dark contrast against a bright background. The additional features now showing between the Nb and Mn columns are the oxygen atom columns. Inset details from each image are shown at the top left, with the arrows pointing to the oxygen columns in the ABF image.

The ordered phases have an-antiferromagnetic transition at 3 K to 5 K. In the crystals that has shown the anti-ferromagnetic transition, both ordered and disordered regions are observed in one crystal piece.

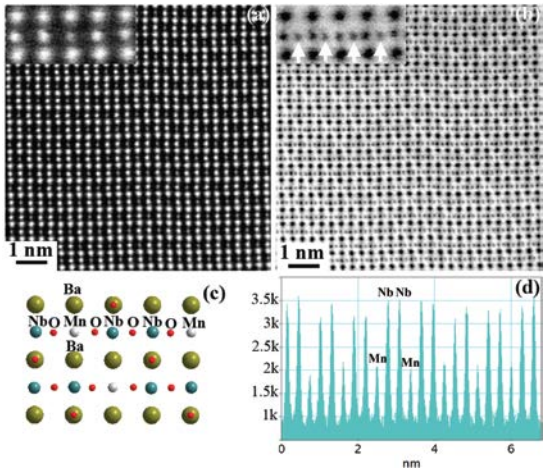

Figure: STEM HAADF Z-contrast image (a) and STEM ABF image (b) of [100] $Ba_3MnNb_2O_9$ single crystal; The insets showing the blown up regions; the oxygen atoms are indicated by arrows; (c) Schematic of the unit cell structure projected along [100]; (d) intensity line profile of the Nb-Mn atomic planes from (a) showing the ordering of ..-Mn-Nb-Nb-Mn-..

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