Corrigendum

H. Sreemoolanadhan, J. Isaac, M. T. Sebastian, K. A. Jose & P. Mohanan: Synthesis, characterisation and properties of $(Ba_{1-x}Sr_x)(Nd_{1/2}Nb_{1/2})O_3$ ceramics for application as dielectric resonators in microwave circuits.

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In this paper we have reported $(Ba_{1-x}Sr_x)(Nd_{1/2}Nb_{1/2})O_3$ is face centred cubic with $(NH_4)_3FeF_6$ structure (page 386). The X-ray diffraction pattern recorded from the samples (Figure 1, *Ceram. Int.*, **21**(6) (1995) p. 386) were in agreement with earlier reports[1–4] and JCPDS File[5] indicating a cubic structure. But more recently it was found[6–8] that the structure of $Ba(Ln_{1/2}Nb_{1/2})O_3$ [Ln = lanthanide] is related to its tolerance factor defined[9] as

$$t = \frac{R_{Ba} + R_O}{\sqrt{2}\left\{\left(\frac{R_{Na} + R_{Nb}}{2}\right) + R_O\right\}}$$

where R is the crystal or ionic radius. The high symmetry phase (cubic) is unstable at room temperature at a tolerance factor less than 0·985 and the resulting phase transition involves tilting of the octahedra in antiphase. At $t = 0{\cdot}965$, a second phase transition occurs which involves tilting of the octahedra in-phase. The complex perovskites with $t < 0{\cdot}985$ are cubic at high temperature and transform to one with a lower symmetry (tetragonal or orthorhombic) on cooling. The transition temperature correlates[8] inversely with tolerance factor. The materials with t in the range 0·985–1·03 do not undergo any phase transition and they have a cubic structure. Recently, $Ba(Nd_{1/2}Nb_{1/2})O_3$ is reported[7] as cubic at high temperature and transforming to tetragonal at 646 K on cooling.[7] In the case of $(Ba_{1-x}Sr_x)(Nd_{1/2}Nb_{1/2})O_3$, t lies in between 0·962 and 0·91, depending on the value of x. Hence, $(Ba_{1-x}Sr_x)(Nd_{1/2}Nb_{1/2})O_3$ is expected to be cubic at high temperature and transform to tetragonal on cooling, with transition temperature inversely depending on the value of the tolerance factor. The lowering of the symmetry in perovskites is due to the tilting of the BO_6 octahedra.[10] X-ray diffraction is largely insensitive to the scattering from the oxygen sublattice and therefore it is difficult to detect structural phase transition. The distortion of the cation sublattice is small and the associated peak splitting may be difficult to observe.[6,7] Hence, the X-ray diffraction studies made by earlier workers[1–5] and ourselves could not identify the correct room temperature structure. In the case of $(Ba_{1-x}Sr_x)(Nd_{1/2}Nb_{1/2})O_3$ our recent careful X-ray diffraction study using a scan rate of 2 deg./min shows peak splitting at higher angles (see Fig. 1). It should be noted that neutron diffraction experiments are needed to find the structure of $(Ba_{1-x}Sr_x)(Nd_{1/2}Nb_{1/2})O_3$ with certainty.

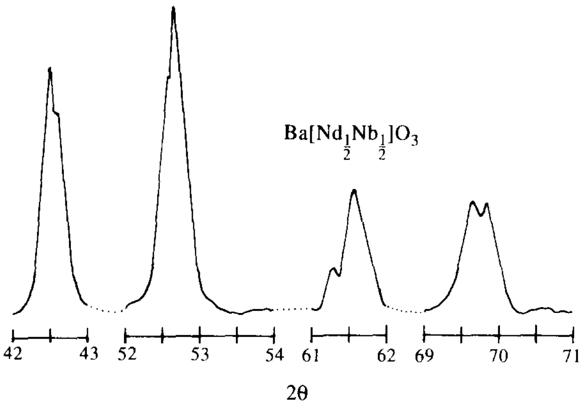

Fig. 1. Powder X-ray diffraction pattern of $Ba(Nd_{1/2},Nb_{1/2})O_3$ ceramic obtained using CuKα radiation, with a scanning rate of 2 deg./min.

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