Poster Presentation

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On the symmetry peculiarities of Bi_2WO_6 single crystals

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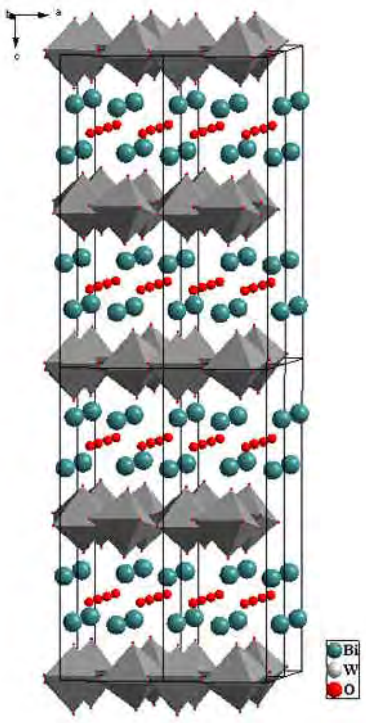
Bi_2WO_6 single crystals (a=5.452(1), b=5.433(1), c=16.435(1) Å) were studied by X-ray diffraction (MoKα radiation, diffractometer Xcalibur S, CCD-detector) and electron diffraction techniques. Bi_2WO_6 is an archetypal x=1 member of the Aurivillius family of layered perovskites of general formula $Bi_2O_2A_{x-1}B_xO_{3x+1}$. Its high piezoelectric performance and nonlinear optical properties have attracted considerable attention. In addition, these crystals offer high ionic conductivity due to the fast oxygen ion transport. In recent years, this compound has been the subject of intense research in the context of catalytic applications. In this work, the Bi_2WO_6 single crystals were grown from solution in melt of Na_2WO_4–NaF. There were reflections with indexes 0kl, k=2n+1, in the diffraction pattern, contradicting the sp.gr. $P2_1ab$. The structure was solved by direct methods and refined in the sp.gr. P1 (R=3.60%, Rw=3.52%). The group $P2_1ab$ was found to describe the arrangement of heavy atoms Bi and W only (R=17.5%, Rw=18.68%). The structure can be described by three local groups of symmetry – each atomic layer has inherent symmetry: W atoms and O atoms in equatorial vertices of WO6-octahedra have P11b sp.gr., Bi atoms – Bm11, the rest of O atoms – B11b. The oxygen atoms between two Bi sheets can be also described by B11m sp.gr. Preliminary electron diffraction investigation of the Bi_2WO_6 crystals indicated a presence of small amount of a minority phase B1a1 together with the main $P2_1ab$ phase. The presence of B1a1 phase can be probably explained by Na content in the crystal originating from the flux. Bi_2WO_6 single crystals were studied earlier [1]. TEM showed coherent intergrowths of two distinct modulated variants having different symmetry. This result couldn't be explained by impurity presence because of investigation of pure crystals grown from melt. The work was done with the partial support of the grant for Leading Scientific Schools NSh-1130.2014.5 and RFBR (proj.14-02-00531a).

[1] *A.D. Rae, J.G. Thompson, R.L. Withers, Acta Cryst., 1991, B47, 870–881*



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