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Phase transition in FeOCl. Jian Zhang, Alexander Wölfel, Liang Li, Sander van Smaalen. *Laboratory of Crystallography, University of Bayreuth, Germany.*
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The crystal structure of the compound FeOCl with the orthorhombic space group $Pmnm$ was determined by Goldshtaub in 1934 [1]. The magnetic phase transition at $T_N \approx 80$ K has been studied by several authors [2-4]. Here, we present temperature-dependent X-ray diffraction studies of this transition. With synchrotron radiation, single-crystal X-ray diffraction was performed at beamline D3 of HASYLAB at DESY (Hamburg, Germany). The paramagnetic to antiferromagnetic transition occurs at 79.77 K in our sample, which is on the lower side of the published values. The phase transition is accompanied by a temperature-dependent monoclinic lattice distortion with $\gamma = 90.079^\circ$ at $T = 10$ K. The phase transition presumably is of second order with a critical exponent $\beta = 0.2293(25)$. Superstructure reflections were found between 10 K and 58 K, which indicate an incommensurate displacive modulation wave accompanying the incommensurate antiferromagnetic order.

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Thermomechanical properties of mullite-type Bi₂M₄O₉ and Bi₂Mn₄O₁₀ compounds. Thomas F. Krenzel^a, Jürgen Schreuer^a, Manfred Burianek^b, Manfred Mühlberg^b, Hartmut Schneider^b. ^a*Institute of Geology, Mineralogy and Geophysics, Ruhr-University Bochum, Germany.* ^b*Institute of Crystallography, University of Cologne, Germany.*
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Orthorhombic mullite-type Bi₂M₄O₉ (M = Al³⁺, Ga³⁺, Fe³⁺) compounds doped with divalent cations like Sr²⁺ substituting Bi³⁺ are supposed to exhibit ion conductivity at elevated temperatures [1]. These compounds are therefore promising candidates for applications in solid oxide fuel cells. The structurally closely related Bi₂Mn₄O₁₀ exhibits multiferroic properties like ferromagnetism and ferroelectricity [2]. Both Bi₂M₄O₉ and Bi₂Mn₄O₁₀ are built up from edge-sharing MO₆ and Mn₄O₆ octahedra forming chains along [001]. In Bi₂Mn₄O₁₀, they are linked by edge-sharing Mn₃O₅ square pyramids which alternate with distorted BiO₅ polyhedra in the (001) plane along the *c* axis. In Bi₂M₄O₉, neighbored chains are linked by M₂O₇ dimers. Parallel to [001] the dimers alternate with structural cavities. The stereochemically active 6s lone electron pairs (LEP) of the adjacent Bi³⁺ cations point towards the centres of these cavities. Therefore the LEPs stabilise the mullite-type structure of Bi₂M₄O₉ compounds [3]. In Bi₂Mn₄O₁₀, however, the cavities are occupied by additional oxygen atoms required for charge compensation reducing the stereochemical activity of the LEPs.

Large single crystals of Bi₂Ga₄O₉, Bi₂Fe₄O₉ and Bi₂Mn₄O₁₀ were grown by the top-seeded solution growth method [4]. In order to study their bonding system we determined the single crystal elastic constants of the Bi-mullites from room temperature to 1173 K using resonant ultrasound spectroscopy.

Additionally, the thermal expansion behaviour was investigated in the same temperature range employing dilatometry. For comparison the elastic properties of 2/1-mullite single and polycrystalline samples were studied. The elastic constants decrease continuously with increasing temperature, showing no evidence of any structural instability. However, all compounds display distinct anelastic relaxation peaks near room temperature, probably caused by point defect relaxation processes. The elastic properties of 2/1-mullite compare well with the behaviour of sillimanite, whereas with respect to elastic anisotropy the Bi-containing compounds resemble andalusite.

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