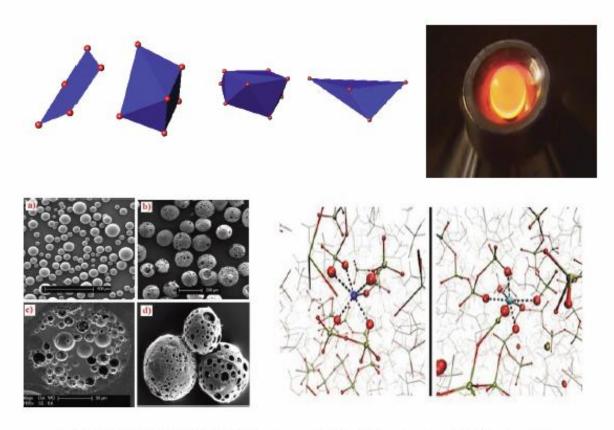
BORATE GLASSES, CRYSTALS AND MELTS:

Ninth International Conference



PHOSPHATE MATERIALS: Second International Conference

St Anne's College, Oxford, UK 24 – 28 July 2017 Borate 9 – Phosphate 2: Abstracts from the Ninth International Conference on Borate Glasses, Crystals & Melts and Second International Conference on Phosphate Materials

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X-Ray diffraction and Mössbauer studies of Fe₃O₂(BO₄) at different temperatures

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Fe₃BO₆ has been investigated intensively in recent years due to its potential applications in nanoceramics [1]. Besides, in a specific shape of nanorods this compound is promising anode element for Li-ion batteries [2] and it is the perfect material for a combination of functional magnetic and dielectric properties in an electrode or a gas sensors [3].

Recently the thermal behavior of Fe₃O₂(BO₄) in the temperature range 20-900°C has been studied using high-temperature X-ray diffraction [4]. Damping of thermal expansion with an increase in temperature has been revealed. One is unusual for thermal expansion and can be explained by the appearance of additional process besides thermal expansion, and physics of this phenomenon isn't clear up to now. In order to control the cations distribution and the microscopic magnetic and electric properties of Fe ions in crystal structure of our Fe₃O₂(BO₄) sample, Mössbauer spectroscopy measurements were conducted.

In the present work the experimental data of Fe₃O₂(BO₄) Mössbauer effect in the temperature range of 80–800 K are presented. In the temperature range below T_N (T<510 K) the hyperfine magnetic field (HF) on Fe nucleus for both crystallographic positions (4c and 8d) is decreased with the temperature growth. Temperature dependence of the isomer shift (IS) for both positions is monotonically decreasing due to the second-order Doppler effect. The quadrupole splitting $\epsilon = \Delta_{12} - \Delta_{56}$, where Δ_{12} and Δ_{56} are the splittings between sextet lines 1, 2 and 5, 6 respectively, shows a evident features at near 400 K and near the Néel temperature. The first jump of ε at ~400 K is caused by the change in the direction of magnetization (spin reorientation), the second one (~510 K) is caused by the transition from the antiferromagnetic to the paramagnetic state. At higher temperatures, two doublets are observed in the spectrum. As the temperature increases, the isomer shift of doublets is monotonically decreases in accordance with the second-order Doppler effect. The change of the quadrupole splitting of doublets is almost linear, but an angle of slope for one position is slightly more than for the other, that may be associated with the damped character of thermal expansion.

The work was supported by the Russian Foundation for Basic Research (grant no. 15-03-05845). The X-ray diffraction experiments were performed at the X-ray Diffraction Centre of St. Petersburg State University.

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