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Neutron diffraction studies of pressure induced phase transitions in Bi2WO6

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Bi2WO6 is the simplest member of the Aurivillius family, but it possesses many interesting physical properties such as ferroelectricity with large spontaneous polarization and high Curie temperature (Tc=960), piezoelectricity with a potential for high-frequency and high temperature applications, high ion conductivity and photocatalytic activity. But apart from potential application, bismuth layered compounds are attractive for great number of scientific research. However, pressure dependent studies of this family of compounds are scarce. It should note, the high pressure studies of the ferroelectric phase evolution, especially in the vicinity of para-ferroelectric phase transition are essential in order to reveal its formation mechanisms upon variation of interatomic distances.

It present work the compound of Bi2WO6 was chosen at ambient condition, and performed neutron diffraction studies at high pressure. Neutron powder diffraction measurements at ambient and high pressures up to 7 GPa were performed at room temperatures with the DN-12 diffractometer at the IBR-2 high-flux pulsed reactor [FLNP, JINR, Dubna, Russia] using the sapphire anvil high-pressure cell. In order to improve the understanding of the lattice instabilities the Raman spectroscopy studies of the vibration spectra of the Bi2WO6 under pressure up to 30 GPa were performed.

The lattice compression of the unit cell is anisotropic with the most compressible of b parameter and weakly compressible a and c lattice parameters. At P≈3.5 GPa anomalies in pressure behavior of lattice parameters were observed, which are affected by the phase transition (from Pca21 to B2cb space group). There are also observed the clear changes of the vibrational modes of Bi2WO6 under compression. By increasing the pressure, wave numbers of the majority of modes increase, however, some modes exhibit negative pressure dependence. Changes in the slope of wave number vs pressure at 3.5 and 6 GPa are observed for a lot of modes, which indicates about a second order phase transitions associated with some subtle changes in the crystal structure. The first transition is most likely associated with the loss of the octahedral tilt mode around the pseudotetragonal axis and the phase symmetry changes from Pca21 to B2cb.The second transition is related to the disappearance of the soft mode. On the dependences of the vibrational modes from 6 to 30 GPa have revealed no anomalies.
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