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Investigation of high pressure phase transition by means of infrared spectroscopy in the Cairo frustrated pentagonal magnet Bi2Fe4O9

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Bi2Fe4O9 is a common by-product in the synthesis of the multiferroic compound BiFeO3 and has been claimed itself to display multiferroic properties [1]. The lattice formed by the two different sites of four iron Fe3+ magnetic atoms is quite remarkable as it materializes the first analogue of a magnetic pentagonal lattice [2]. For its peculiar lattice geometry it has attracted interest in the field of geometrical frustration. At room temperature and atmospheric pressure, the crystal structure is orthorhombic within the Pbam space-group and the compounds undergoes a magnetic phase transition at 238 K from a paramagnetic state toward a non collinear magnetic state characterized by a propagation vector k = (1/2,1/2,1/2) and a large degree of frustration (θp/TN ~ 7) [2]. Recently it has been shown that Bi2Fe4O9 undergoes a structural transition under pressure at 6-8 GPa toward the maximal non-isomorphic subgroup Pbnm, with c'= 2c. The driving force of the phase transition is the displacement of the O1 oxygen atom from fully constrained Wyckoff position 2b to a less-constrained 4c one [3]. Previous studies have reported the investigation of dynamical properties by mean of Raman spectroscopy both at ambient condition and at high pressure in a diamond anvil cell [3,4]. However, the vibrational modes involving O1 oxygen atoms are not Raman active but infrared active.
We will report the first polarized infrared spectroscopy measurement of Bi2Fe4O9 performed in a DAC from 1 to 20 GPa in the far-infrared range [60-800 cm-1] and at low temperature. The measurements have been performed at the AILES beamline of synchrotron SOLEIL exploiting the high-pressure/low-temperature set-up [5] coupled with the high brilliance of the radiation source in a wide spectral range on a very thin sample (~50 μm) placed between diamonds with culets of 500 μm diameter. From our high quality spectra, we are able to identify the B3u and B2u modes within the (ab)-plane. Interestingly, while all phonon frequencies increase with pressure, the phonon mode around 200 cm-1 undergoes an anomalous softening with increasing pressure. In order to assign the phonon modes and reveal the microscopic mechanism of the high-pressure transition we also have performed DFT calculation at different pressures. The calculation mostly accounts for the measured phonon modes allowing the assignation of atomic motions.

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Summary

Topic

1. Materials under high pressure

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