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Multiple Phase Transitions in the model multiferroic BiFeO3

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Bismuth ferrite BiFeO3 (BFO) is commonly considered a model system for multiferroics, and is perhaps the only material that is both magnetic and a ferroelectric with a strong electric polarization at 300K [1]. Despite numerous investigations, the crystal structures of BFO as a function of temperature and pressure are still not established and lead to ongoing controversial reports in the literature [1,3]. Besides being a model multiferroic, BFO is also one of the very few materials that present both octahedra tilts and strong cation displacements at room temperature. Here we report the high-pressure phase transitions in BFO by both synchrotron x-ray diffraction and Raman spectroscopy, namely a surprising richness of six phase transitions in the 0–60 GPa range [2-3]. At low pressures, 4 transitions are evidenced at 4, 6, 7 and 11 GPa. In this range, the crystals display in that range unusual large unit cells and complex domain structures, which suggests a competition between complex tilt systems and possibly off-center cation displacements. The non polar Pnma phase remains stable over a large pressure range between 11 and 38 GPa. The two high pressure phase transitions at 38 and 48 GPa are marked by the occurrence of larger unit cells and an increase of the distortion away from the cubic parent perovskite cell. The previously reported insulator-to-metal transition appears to be symmetry breaking. Finally, we will present a new schematic P-T phase diagram for BFO and discuss the recently reported phase transition in highly strained BFO films [4,5] in the light of our high-pressure findings.

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