Stabilization and switchability of weak ferromagnetism in epitaxially strained $BiFeO_3$

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The magnetoelectric effect (ME), i.e. controlling ferromagnetism using electric fields, has been a focus of research in multiferroic materials due to potential applications in technologies such as magnetic data storage, spintronics, logic and memory devices[1,2]. Magnetoelectric coupling with substantial magnetic stability and switchability is critical for magnetic information processing with minimal power consumption. In this regard, bismuth ferrite ($BiFeO_3$), has been shown to exhibit coupling between the ferroelectricity and ferromagnetism[3]. Here, we show the stabilization and the swichability of weak ferromagnetism (wFM) under epitaxial strains in $BiFeO_3$ using a first-principles approach and group-theoretic analysis. For this purpose, we perform non-collinear spin-polarized density functional theory (DFT) calculations including spin-orbit couplings under applied compressive and tensile strains. In case of rhombohedral symmetry, we observe that the magnetic ground state is degenerate (refer Figure 1) and is perpendicular to the polarization vector, which is a consequence of isotropic Dzyaloshinskii-Moria interactions. Such degeneracy, however, disappears for the strained phases.

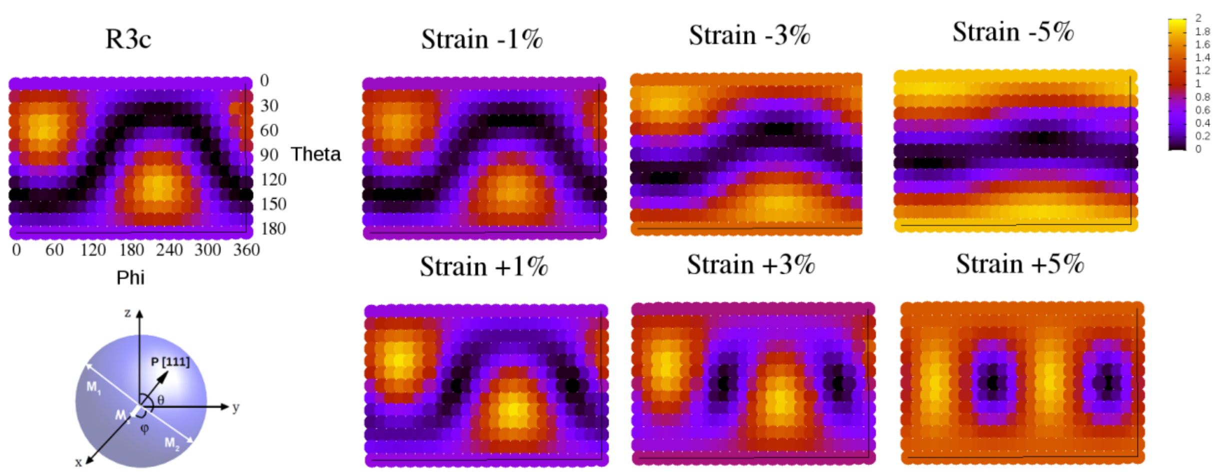

Figure 1. Calculated magnetic energy landscapes showing the energy difference (in meV) between the antiferromagnetic arrangements considered along all the possible orientations in space. The bright spots coincide with the direction of the polarization vector and the dark region represents the magnetic ground state (remains perpendicular to the polarization vector in all the cases).

We find that the tensile strain can be used to stabilize the antiferromagnetic vector along the [1-10] direction due to anisotropic Dzyaloshinskii-Moria interactions in the x-y plane, commensurate with changes in the FeO_6 octahedral tilt pattern. On the other hand, at high enough compressive strains the *C* and *G*-type magnetic ordering are energetically indistinguishable from each other. Furthermore, *C*-type magnetic ordering shows weak antiferromagnetism (wAFM), i.e. the wFM moments are antiferomagnetically ordered in the neighboring planes. Thus it may be possible to switch “on” and “off” the wFM at higher compressive strains.

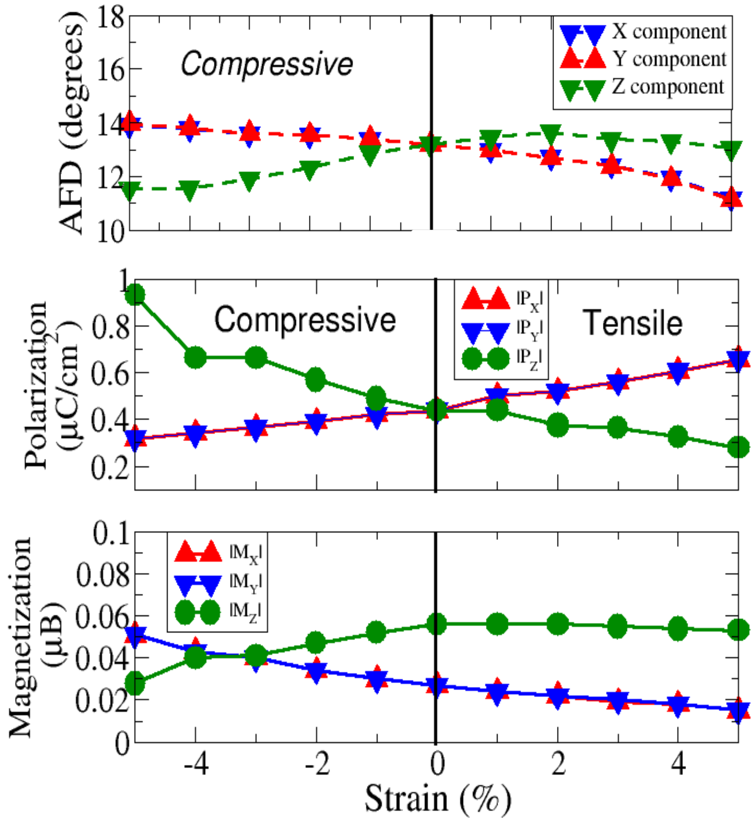

Figure 2. Variation in the in-plane (x-y) and out-plane (z) components of the antiferrodistortive (AFD)rotations polarization (P) and magnetization (M) under applied epitaxial strain.

Finally we summarize the relation between the antiferrodistortive (AFD) rotations and ferroelectric polarization (P) and weak ferromagnetic moment (M) induced via the DM interactions (Figure 2). Our study shows that the wFM is directly linked to the amplitude of AFDs and epitaxial strain is a powerful tool to manipulate the ME coupling in $BiFeO_3$ thin films.

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References

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