Strain effect on Magnetocrystalline Anisotropy of Multiferroic Fe/$BaTiO_3$

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Using the highly precise full-potential linearized augmented plane-wave method within general gradient approximation, we studied the magnetism of Fe monolayer on $BaTiO_3$ (BTO), which has been recently expected as a multiferroic heterostructure. As previously predicted with the pseudo-potential method [C.G. Duan *et al.,* Phys. Rev. Lett. 97, 047201 (2006), Appl. Phys. Lett. 92, 122905 (2008)], we approved that the ferroelectric Ti polarization alters significantly the magnetic moment and magneto-crystalline anisotropy energy (EMCA) of Fe/BTO. In addition to the change of EMCA due to the electric polarization, it is also found to be very sensitive to substrate strains. As the compressive strain is applied, the calculated EMCA decreases from 1.4 meV/Fe at the lattice constant (3.991 Å) of BTO to 1 meV/Fe at the compressive strain of 2.2 % which corresponds to the lattice of SrTiO3 (STO). Whereas, the tensile strain increases the EMCA and large value of 2 meV/Fe is obtained at the tensile strain of 3 %. Magnetic moments of Fe and Ti atoms reduce (increases) slightly as the compressive (tensile) strain increases. An example model of Fe/BTO/STO in this study reveals that the changes of magnetization ofa ferromagnet in response to the ferroelectric polarization across the interfacecan also be manipulated by the lattice strain with a suitable third alien.