First-principles calculations of multiferroic interfaces

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To obtain large magnetoelectric coupling in multiferroic materials, multiferroic interfaces are promising, because single-phase multiferroic materials exhibit typically antiferromagnetism preventing from having net magnetization [1, 2]. In addition to multiferroic interfaces, many types of magnetic interfaces are of fundamental importance to enhance the performance of magnetic materials. Nevertheless, our understanding from electron theory is far from being satisfactory. Since first-principles calculations of magnetic interfaces are computationally challenging, such study is also of importance in the sense of large scale computations.

In this project, we performed first-principles calculations of magnetic interfaces related with multiferroic materials [3–5] and permanent magnets [6–8]. We demonstrated enhancement of magnetoelectric coupling by insertion of Co atomic layer into $Fe_3Si/BaTiO_3(001)$ interfaces from first principles [3]. As is shown in Fig. 1, the interface Co monolayer helps the interface ferroelectric polarization exhibit enough, whereas the interface electric polarization is killed by Si without the Co monolayer at the interface. Other transition-metal monolayers are also investigated [4]. In addition, crystal-growth mechanism was also clarified for Co_2FeSi and Co_2MnSi films on single-crystalline oxides by identifying the initial disorder at the deposition and the formation energy of random alloys relative to ordered alloy [5] by using both of OpenMX [9] and Akai-KKR [10]. Substantial progresses were obtained also for microstructure interfaces in permanent magnets [6–8].

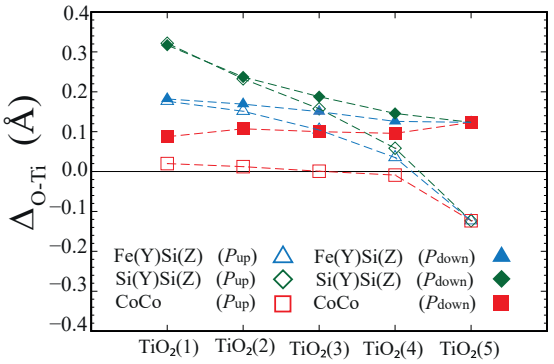

Figure 1: Relative displacements $\Delta_{O-Ti} = z_O - z_{Ti}$ in the tetragonal $BaTiO_3(001)$ film for each interface. For the Fe(Y)Si(Z) case, average values for Δ_{O-Ti} are shown. The first layer $TiO_2(1)$ is the interface layer, whereas the fifth layer $TiO_2(5)$ has the bulk atomic positions of $BaTiO_3$.

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