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論 文 要 約

THESIS OUTLINE

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First-principles study of multiferroic composite with strain transfer

(歪み移動を伴うマルチフェロイク複合材料の第一原理的研究)

The thesis entitled "**First-principles study of multiferroic composite with strain transfer**" consists of five chapters in English.

Chapter 1, "**Introduction**," introduces past research and issues related to multiferroic composites consisting of ferroelectric and ferromagnetic materials. In order to increase the magnetoelectric coupling coefficient, it is effective to use a mechanism in which ferroelectric polarization controlled by an electric field induces interfacial strain, where the strain modulates the magnetic anisotropy of the ferromagnetic phase. We pointed out that the single-phase magnetic anisotropy modulation mechanism has not been fully clarified yet, and that the separation of bulk and interfacial effects in multiferroic composites has not been analyzed. The aim of this thesis is to prove that quantum mechanical second-order perturbation theory is effective for elucidating the mechanism of magnetic anisotropy modulation in the multiferroic composite, and that simulations for junction systems, rather than single phases, are effective for separating bulk and interfacial effects.

Chapter 2, "**Basic theory and computational methods**," describes the theoretical framework used in this study. The key points of numerical analysis methods for magnetic anisotropy analysis incorporating first-principles electron theory and spin-orbit interaction were described.

In Chapter 3, "**Origin of modulated magnetic anisotropy in single-phase Heusler alloys,**" the Heusler alloys Co_2FeSi, Co_2MnSi, and Fe_3Si are used as examples to study the mechanism of strain-induced magnetic anisotropy in single-phase ferromagnets. The selected alloys were used in experiment for multiferroic composites as the ferromagnetic components and demonstrated strong magnetoelectric coupling coefficients which related to the magnetic anisotropy modulation in the alloys. However, the mechanism has not been fully understood yet. From the theoretical analysis applying second-order perturbation theory, the conventional framework of the orbital magnetic moment and the quadrupole moment of electron density is considered to be the orbital angular momentum in the spin-orbit interaction and the off-diagonal component of the spin angular momentum. By using this approach, the main contributing factors of strain-induced magnetic anisotropy for Co_2FeSi and Co_2MnSi were successfully evaluated where the contribution from Co atoms are dominant. However, it was clarified that for some Heusler alloys, such as Fe_3Si, this approach is qualitatively and quantitatively inadequate because some of the electronic state modulations due to spin-orbit interaction have been neglected. It is pointed out that it is important to incorporate all virtual excitations in spin invariance and reversal in the second-order perturbation as a more precise theoretical analysis method than the conventional method.

In Chapter 4, "**Magnetoelastic effect in multiferroic composite by domain modification,**" a large-scale first-principles calculation incorporating spin-orbit interaction is presented for a multiferroic composite material, which is a ferromagnetic/ferroelectric junction system. We simulated the interface effect that cannot be described by the single-phase bulk effect. First, we discuss the stability of the interface, and theoretically analyze the modulation of the magnetic anisotropy due to the change in the ferroelectric domain for the interface identified as stable. The in-plane uniaxial magnetic anisotropy of Co_2FeSi was observed when the ferroelectric domains were polarized parallel to the interface, whereas the magnetization was significantly different in the plane for the electrical polarization perpendicular to the interface. It turned out that the magnetization can be easily rotated. While the main part of the modulation of the magnetic anisotropy is dominated by the single-phase effect as the bulk effect, symmetry breaking due to the interfacial effect was observed in the ferromagnetic ultrathin films. The origin of the modulated magnetic anisotropy can be attributed to the shifting of specific energy band in Co_2FeSi when the ferroelectric domain is modified.

Chapter 5, "**Conclusion**," summarizes this thesis and discusses future prospects. In summary, we clarified the magnetic anisotropy modulation mechanism in multiferroic composites, pointed out the limitations of the existing theoretical framework, and proposed a more precise analysis method. Furthermore, it was shown that the magnetoelectric coupling can be modulated by the interfacial effect by making the ferromagnet on the ferroelectric thinner. These results provide basic knowledge that contributes to further functional improvement of multiferroic composites, and contribute greatly to the development of theories describing magnetic anisotropy and multiferroic composites. Based on the knowledge provided in this thesis, we would like to mention possible future study on the strain-induced orbital and quadrupole moments modulation in both of single-phase Heusler alloys and multiferroic composites by using first-principles X-ray spectroscopy simulations. In recent experiment, X-ray magnetic circular dichroism (XMCD) spectroscopy measurement has been used to detect the significant contribution of the orbital moment in Fe to the total magnetic anisotropy modulation in the Co_2FeSi-based multiferroic composite which is different to our findings, where the crystal orientation of Co_2FeSi in the experiment is different to that in our study. Clarifying the underlying mechanism of this differences will be benefit for the material designs focusing on functional improvement of multiferroic composites.