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題目(和文)	ペロブスカイト型酸化物における3d電子配置の変化を用いた物性と結晶構造歪みの制御
Title(English)	Electronic configuration control of 3d transition metal in perovskite oxides for tuning physical properties and structural distortion
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Summary of
**“Electronic configuration control of
3d transition metal in perovskite oxides for tuning physical properties
and structural distortion”**

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In this thesis, I showed three examples of materials design based on the electronic configuration control of 3d transition metals in Bi or Pb - 3d transition metal perovskites. The interesting findings are as follows:

1. Demonstration of electric field induced reorientation of magnetic easy plane in Co-substituted BiFeO₃
2. Demonstration of the strong electron-lattice coupling and colossal negative thermal expansion in a giant tetragonal perovskite
3. Synthesis of new lead-free tetragonal perovskite Bi_{0.5}Na_{0.5}VO₃ and Bi_{0.5}K_{0.5}VO₃ with moderate *c/a* ratios and spontaneous polarizations

In chapter 2, the spin structure change and the strong coupling between weak-ferromagnetism and spontaneous polarization P_S via Dzyaloshinskii-Moriya interaction in Co-substitute BiFeO₃ were studied. In order to study the magnetoelectric coupling, BiFe_{0.9}Co_{0.1}O₃ and BiFe_{0.892}Mn_{0.008}Co_{0.1}O₃ single crystals were grown at high pressure condition. Electric field induced reorientation of magnetic easy plane were demonstrated by means of remanent magnetization measurement on the single crystals. This result is the first demonstration of an electric field affecting the local magnetic moment of Co-substituted BiFeO₃.

In chapter 3, the strong electron-lattice coupling via Jahn-Teller effect in a giant tetragonal perovskite vanadate were studied. A structural transition from tetragonal-to-cubic structure was accompanied by a colossal volume collapse of 6-8 %, which is the largest volume contraction among oxide materials. I found that filling control is an

effective way to realize a negative thermal expansion materials based on giant-tetragonal perovskites.

In chapter 4, new tetragonal perovskites, $\text{Bi}_{0.5}\text{Na}_{0.5}\text{VO}_3$ and $\text{Bi}_{0.5}\text{K}_{0.5}\text{VO}_3$, were designed based on the idea of cooperating between an optimized stereo-chemical effect on the *A*-site and a Jahn-Teller effect on the *B*-site cation. The tetragonal perovskites $\text{Bi}_{0.5}\text{Na}_{0.5}\text{VO}_3$ and $\text{Bi}_{0.5}\text{K}_{0.5}\text{VO}_3$ were successfully synthesized at 6 GPa and 1200°C for 30 min. The magnitudes of *c/a* ratio and P_S were comparable to those of PbTiO_3 , $c/a = 1.085$ and $P_S = 73 \mu\text{C}/\text{cm}^2$ for $\text{Bi}_{0.5}\text{Na}_{0.5}\text{VO}_3$ and $c/a = 1.054$ and $P_S = 55 \mu\text{C}/\text{cm}^2$ for $\text{Bi}_{0.5}\text{K}_{0.5}\text{VO}_3$, respectively. Magnetic and electric properties indicated the lifting of the t_{2g} degeneracy and $3d_{xy}$ orbital ordering caused by a Jahn-Teller effect as in PbVO_3 . These results provide a guideline to design new lead-free ferroelectric and piezoelectric materials, cooperation of an optimized *A*-site and Jahn-Teller active *B*-site cation possessing $3d^1$ (or $3d^6$) electronic configuration.

In conclusion, the findings of this thesis would lead to the development of new functional materials, including multiferroics, negative thermal expansion materials and lead-free ferroelectrics and piezoelectrics.