第122 回フロンティア材料研究所講演会

講師：Dr Y. K. Wakabayashi　若林勇希博士
NTT Basic Research Laboratories　NTT物性科学基礎研究所

1月28日（火）　15時～　R3棟6階セミナー室にて

演題：Molecular beam epitaxy and utilization of machine learning for development of novel and high-quality 4*d* and 5*d* magnetic oxides

Magnetic oxides are typically 3*d* transition metal oxides where spin-orbit coupling (SOC) is tiny, while an enhancement of the SOC in 4*d* and 5*d* systems may enrich variety of fascinating magnetic materials. Recently, we have developed a novel 5*d* perovskite Sr_3OsO_6 (FM insulator) and improved the material quality of a 4*d* perovskite $SrRuO_3$ (FM metal) by using a unique molecular beam epitaxy (MBE) technique.

First, we show that the highly B-site ordered cubic double-perovskite Sr_3OsO_6 has the highest Curie temperature (T_C) of ~1060 K among all insulators and oxides[1] (Fig. 1). Resistivity and optical measurements revealed that Sr_3OsO_6 is an insulator with the band gap of 2.65 eV. Density-functional-theory calculations also elucidated the ferromagnetic ground state of Sr_3OsO_6, where the large SOC of the Os^{6+} $5d^2$ orbitals drives the system toward an insulating state with J_{eff} = 3/2. Sr_3OsO_6 is expected to be readily implemented in high-performance magnetic devices that work above room temperature.

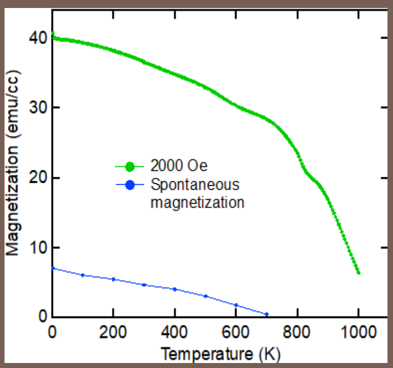

Fig. 1. Magnetization as a function of temperature with H = 2000 Oe for a Sr_3OsO_6 film. Spontaneous magnetization as a function of temperature is also shown.

Second, we demonstrate a machine-learning-assisted MBE growth of $SrRuO_3$[2,3]. To simplify the intricate search space of entangled growth conditions, we ran the Bayesian optimization (BO) for a single growth condition while keeping the other growth conditions fixed. As a result, a high-crystalline-quality $SrRuO_3$ film exhibiting a high residual resistivity ratio (RRR) of over 50 as well as strong perpendicular magnetic anisotropy was developed in only 24 MBE growth runs. Our BO-based search method provides an efficient experimental design that is not as dependent on the experience and skills of individual researchers, and it reduces experimental time and cost, which will accelerate materials research.

References: 1) Y. K. Wakabayashi, et al., Nat. Commun. **10**, 535 (2019).
2) Y. K. Wakabayashi, et al., Appl. Phys. Express **11**, 112401 (2018).
3) Y. K. Wakabayashi, et al., APL Materials **7**, 101114 (2019).

連絡先：東・山本研究室（5315）