

Poster Presentation

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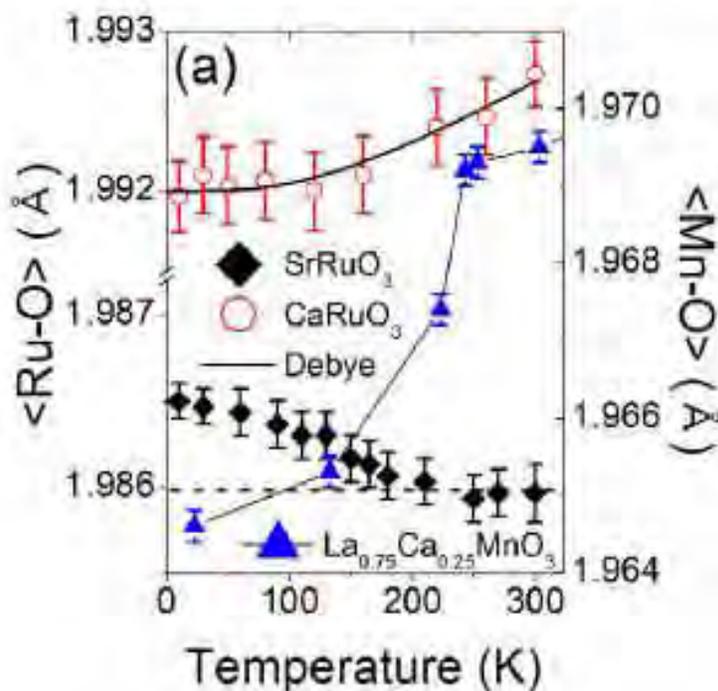
Large in-plane deformation of RuO6 octahedron and ferromagnetism of bulk SrRuO3

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Glazer tilting system with tilting and rotation of oxygen octahedron, can describe ABO₃ perovskite structure effectively. In highest symmetry, Pm-3m(No. 221) crystal structure is a0a0a0 without tilting and rotation. If temperature is lower, the different atomic radius of A and B causes tilting and rotation of BO₆ octahedron. Glazer tiling notation of Pbnm(No. 62, cab lattice) orthorhombic structure is a-a-c+ with antiphase tilting along [110]cubic and in-phase rotation along [001]cubic for neighboring octahedron. SrRuO₃ is rare example of itinerant ferromagnetic among 4d oxides. It shows zero thermal expansion, so called Invar effect below ferromagnetic transition(T_c=165 K). Otherwise, paramagnetic CaRuO₃ has same Pbnm crystal structure without magnetic transition. To understand Invar effect and ferromagnetism of SrRuO₃, We carried out high resolution Time-of-flight powder neutron diffraction using SuperHRPD beamline in J-PARC, with the best resolution Δd/d=0.03% of backscattering bank. Itinerant ferromagnetic SrRuO₃ shows 50 femtometer increase of <Ru-O> mean bond below ferromagnetic transition while paramagnetic CaRuO₃ shows decrease of <Ru-O> and follows well by the usual thermal expansion. For SrRuO₃, Glazer tilting with deformation of RuO₆ octahedron explains Invar effect and why lattice a is larger than lattice b in Pbnm structure. The increased <Ru-O> mean bond is considered as coupled order parameter with ferromagnetic transition. The band width of CaRuO₃ is almost constant in the whole temperature range whereas ones of SrRuO₃ decrease at low temperature. Then more localized Ru 4d orbitals probably contribute ferromagnetic transition.

[1] Sanghyun Lee, J R Zhang, S. Torii, et al., J. Phys.: Condens. Matter 25 482885 (2013)



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