(8a2)

Superlattice structure as a combination of crystal-field states and atomic displacements in the insulator phase of $PrRu_4P_{12}$

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$PrRu_4P_{12}$ undergoes a metal-insulator (M-I) transition at $T_{M-I} = 63$ K (C. Sekine *et al.*: Phys. Rev. Lett. **79**, 3218 (1997)). A structural superlattice due to Ru- and P-atom displacements appears below T_{M-I} (C. H. Lee *et al.*: J. Phys.: Condens. Matter **13**, L45 (2001), C. H. Lee *et al.*: J. Magn. Magn. Mater. **272 – 276**, 426 (2004), L. Hao *et al.*: J. Magn. Magn. Mater. **272 – 276**, e271 (2004)). The high-temperature structure (space group $Im\bar{3}$) depicted in the lefthand side of Fig. 1 transforms to the low-temperature one ($Pm\bar{3}$) shown in the right figure. It is consistent with the charge density wave transition due to the Fermi surface nesting proposed in the band calculation study (H. Harima and K. Takegahara: Physica B **312 – 313**, 843 (2002)). Inelastic neutron scattering study revealed the strong evolution of the crystal-field (CF) state of Pr^{3+}-ion $4f^2$ electrons on the M-I transition (K. Iwasa *et al.*: to appear in Physica B and submitted to Phys. Rev. Lett.). Above T_{M-I}, the inelastic spectrum is significantly broad and all CF ground state is Γ_1. The spectrum below T_{M-I} is reproduced by the the two different CF schemes, and the excitation-peak widths become sharp with decreasing temperature. Below about 40 K, a half of CF ground state switches to $\Gamma_4^{(2)}$. Such evolution can be interpreted by a p-f hybridization effect which enhances the Fermi-surface density of states and causes the M-I transition.

The novel contribution of the 4f electrons to the M-I transition of $PrRu_4P_{12}$ will be understood based on the detailed superlattice structure. In order to investigate the mutual configuration between the superlattice of the atomic displacements and that of the CF states, we carried out a polarized neutron diffraction experiment for a single-crystal sample. Pr ions with the CF scheme with a ground state Γ_1 is located at the sites to which the Ru ions displace closer, and another Pr ions have the CF scheme with $\Gamma_4^{(2)}$ ground state. The superlattice formation of the Pr-ion CF states can be described by the competitive potentials due to the p-f hybridization and the point-charge Coulomb interaction which vary with the change of carrier state and the structural transformation (J. Otsuki *et al.*: private communication).

This study is based on the collaboration with the group of Tokyo Metropolitan University.

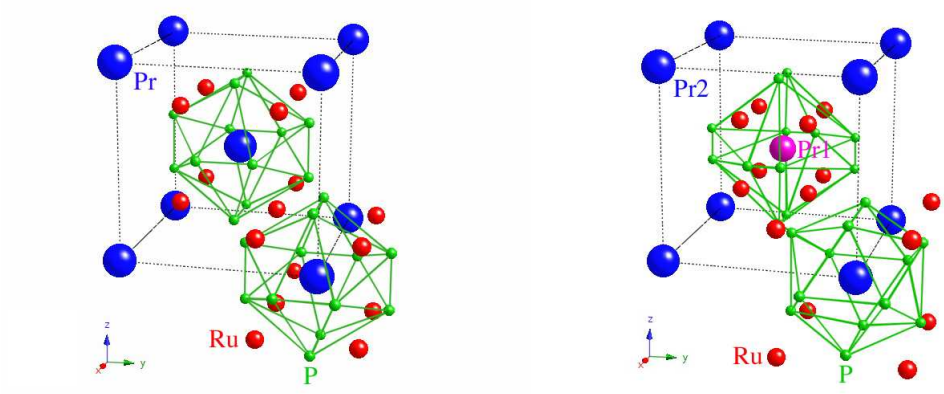

Figure 1: Schematic drawings of the crystal structures in the metallic phase (left) and in the insulator phase (right) of $PrRu_4P_{12}$. Pr1 and Pr2 indicate the Pr ions with the ground state Γ_1 and $\Gamma_4^{(2)}$, respectively. Atomic displacements of Ru and P are emphasized by a hundred times.