PA01

Ferromagnetic filled skutterudites KFe_4Sb_{12} and $NaFe_4Sb_{12}$: Evidence for a high spin polarization

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The chemical, structural, and magnetic properties of alkali-metal compounds with filled-skutterudite structure, $NaFe_4Sb_{12}$ and KFe_4Sb_{12}, are described [1,2]. X-ray and neutron diffraction and elemental analysis established the crystal structure without defects and disorder on the cation site. The electronic structure is calculated by LMTO and FPLO methods. Quantum chemical calculations [2] (electron localization function, ELF) reveal the covalent character of both Fe–Sb and Sb–Sb interactions. Electronic structure calculations within the local density approximation (LDA) exhibit a band ferromagnetic ground state and predict a half-metallic behavior [2].

In contrast to isostructural alkaline-earth and ytterbium compounds (Ca, Ba and $YbFe_4Sb_{12}$ [2,3]), the alkali-metal skutterudites are itinerant electron ferromagnets with small magnetic moments ($\approx 0.25\,\mu_B$/Fe atom) and $T_C \approx 85$ K.

Temperature dependent ^{57}Fe and ^{121}Sb Mössbauer spectroscopy confirm the ferromagnetic state in the sodium compound with very small hyperfine fields at the iron and antimony sites [2].

The spin polarization of the compounds is studied by point-contact Andreev reflection using superconducting Nb and Pb tips [4]. From these measurements an intrinsic transport spin polarization of 67% and 60% for the K and Na compound, respectively, is inferred which establishes these materials as a new class of highly spin polarized ferromagnets.

The results are in accord with the band structure calculations that predict nearly 100% spin polarization in the density of states. We discuss the impact of calculated Fermi velocities and spin fluctuations on the transport spin polarization [4].

[1] A. Leithe-Jasper *et al.* Phys. Rev. Lett. 91, 037208 (2003).
[2] A. Leithe-Jasper *et al.* Phys. Rev. B 70, 214418 (2004).
[3] W. Schnelle *et al.* Phys. Rev. B 72, 020402 (2005).
[4] G. Sheet *et al.*, to be published.

PA02

Magnetic and thermoelectric properties of AT_4Sb_{12} (A = Ca, Sr, Ba; T = Fe, Ru, Os)

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Alkali-metal- and alkaline-earth-filled skutterudites AFe_4Sb_{12} (A = Na, K, Ca, Sr, Ba) are attracting much attention because the compounds with monovalent Na and K are itinerant ferromagnets while those with divalent Ca, Sr, and Ba are nearly ferromagnetic systems [1-3]. In the latter, the presence of Fe $3d$ derived flat bands near the Fermi level is manifested in the rather large value of the specific heat coefficient $\gamma = 100$ mJ/K^{2}mol. The characteristic temperature of spin fluctuations was estimated to be 50 K from the maximum in both the magnetic susceptibility χ and thermopower [3]. At lower temperatures, the $(1/T_1T)_{spin}$ measured by Sb NQR in AFe_4Sb_{12} (A=Sr, Ba) goes to zero, which is however unexpected in nearly ferromagnetic systems [4].

In order to understand the unusual magnetic properties of the Fe compounds, we have studied the magnetic and thermoelectric properties of the Ru and Os compounds AT_4Sb_{12} (A = Sr, Ba; T = Ru, Os) [5]. The dense samples were prepared by the spark-plasma sintering method. As is shown in the figure, the χ of the Ru compounds is negative. This diamagnetic behavior is consistent with the small γ value of 10 mJ/K^{2}mol. The magnitude of χ for the Os compounds is one tenth of that of the Fe compounds and its temperature dependence is much weaker compared with the Curie-Weiss behavior. We note that $\chi(T)$ is describable by the form predicted for a strongly coupled electron-phonon system [6,7]. The moderately high value of $\gamma = 45$mJ/K^{2}mol indicates the presence of a large density of states derived from Os $5d$ states near the Fermi level.

The analysis of the thermal conductivity measurements shows that the lattice thermal conductivity κ_{ph} for the Os compounds does not show a peak near 50 K and its value is much smaller than those of the Fe- and Ru-counterparts. This unusual behaviour of κ_{ph} is attributed to the phonon scattering by localized vibrations of A^{2+} ions in the oversized cage of Os_4Sb_{12}. We propose that the strong electron-phonon interaction in the presence of tunneling states is the origin for the shoulder observed in the electrical resistivity around 100 K.

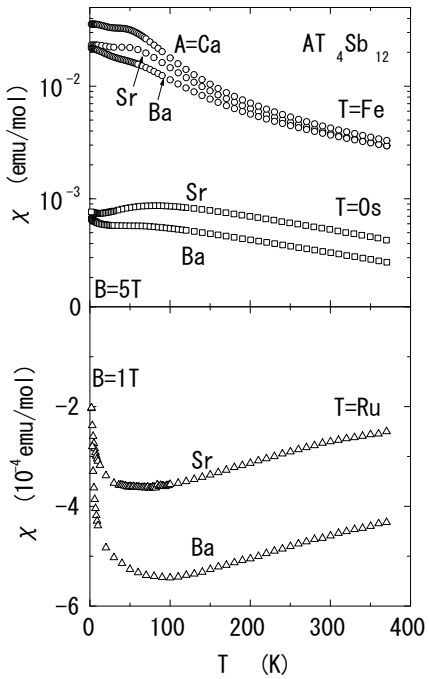

Figure 1: Temperature dependence of the magnetic susceptibility.

[1] A. Leithe-Jasper et al., Phys. Rev. Lett. 91 (2003) 037208.
[2] A. Leithe-Jasper et al., Phys. Rev. B 70 (2004) 214418.
[3] E. Matsuoka et al., J. Phys. Soc. Jpn. 74 (2005) 1382.
[4] M. Matsumura et al., J. Phys. Soc. Jpn. 74 (2005) 2205.
[5] E. Matsuoka et al., submitted to J. Phys. Soc. Jpn.
[6] H. Kusunose et al. Phys. Rev. Lett. 76 (1996) 271.
[7] H. Kusunose et al. J. Phys. Soc. Jpn. 65 (1996) 3032.

PA03

Electronic Band Structures for Alkaline-Earth-Filled Skutterudites

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$NaFe_4Sb_{12}$ and KFe_4Sb_{12} have been known to be a weak itinerant ferromagnet with T_C of 85 K [1,2]. Recently, AFe_4Sb_{12} (A = Ca, Sr and Ba) have been reported to be a nearly ferromagnetic metal [3]. In order to clarify the origin of ferromagnetism, the ferromagnetic energy band structures are calculated by the self-consistent FLAPW method. In the self-consistent iteration processes, we have started with ferromagnetic initial states. Then we have a stable ferromagnetic solution for AFe_4Sb_{12} (A = Na, Ca, Sr, Ba and La), while we can not get a stable ferromagnetic solution for ARu_4Sb_{12} (A = Sr and Ba). These results reveal that the Fe 3*d* band in the vicinity of the Fermi level, which is weakly hybridized with the Sb 5*p* band, induces a ferromagnetic ground state. Note that, among the filled skutterudites, the Fe-Sb skutterudite has the shallowest *d* band and the weakest *p*-*d* hybridization.

Nonmagnetic band structures are also calculated and one of resultant band structures is shown in Fig. 1. Our results of band calculations are consistent with the experimentally measured optical conductivity spectra for $SrFe_4Sb_{12}$ and $SrRu_4Sb_{12}$[4] and the asymmetry parameters η of Sb NQR measurement for $SrFe_4Sb_{12}$ and $BaFe_4Sb_{12}$[5].

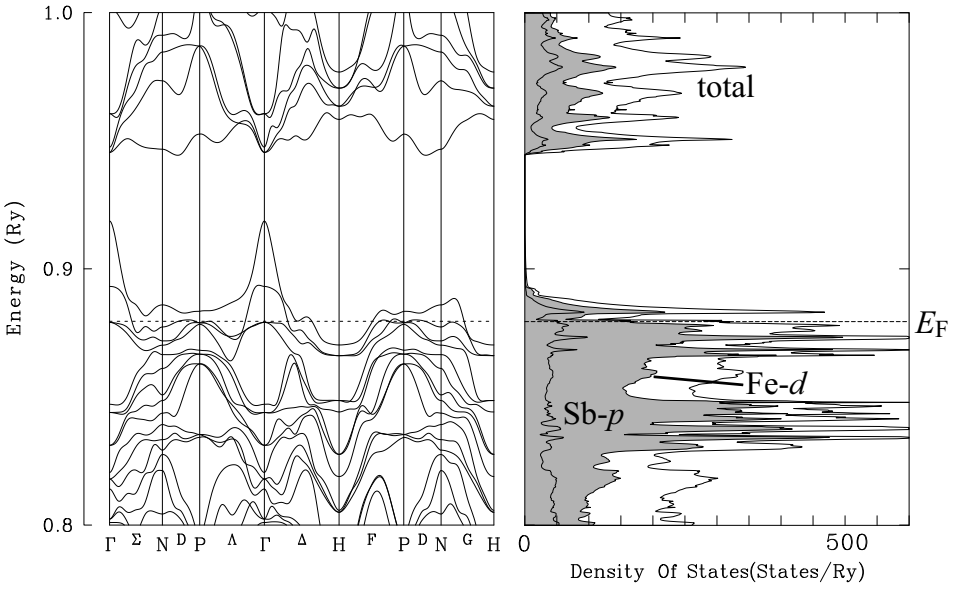

Figure 1: The FLAPW energy band structure and calculated total and partial densities of states for $SrFe_4Sb_{12}$. The Fermi level is denoted by E_F. Total and partial densities of states are the values per F.U.

[1] A. Leithe-Jasper *et al.*, Phys. Rev. Letter **91**, (2003) 037208. [2] A. Leithe-Jasper *et al.*, Phys. Rev. B **70**, (2004) 214418. [3] E. Matsuoka *et al.*, J. Phys. Soc. Jpn. **74**, (2005) 1382. [4] S. Kimura *et al.*, Proc. the 3rd Hiroshima Workshop (2005). [5] M. Matsumura *et al.*, J. Phys. Soc. Jpn. **74**, (2005) 2205.

PA04

Novel Low Temperature Specific Heat Anomaly in Filled Skutterudite Superconductor $LaOs_4P_{12}$

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Filled skutterudite phosphide $LaOs_4P_{12}$ synthesized at high temperatures and high pressures has been studied by specific heat $C(T)$ measurements in magnetic fields. Figure 1 shows a specific heat divided by temperature C/T of $LaOs_4P_{12}$ in various magnetic fields. $LaOs_4P_{12}$ shows a superconducting transition at T_c=1.95 K which is slightly higher than that in previous report [1]. Interestingly, we found the upturn of C/T below 2 K in the normal state; $H_{c2}(0)$ is estimated to be 1240 G from the field dependence of T_c. The upturn is not affected by applying a magnetic field. From the analysis on Zeeman and quadrupole splitting of nuclear spin, we found that this upturn is not caused by a nuclear Schottky anomaly. In addition, the anomalous contribution on C/T shows the temperature dependence of T^{-2}. We should notice that it is different from the high temperature behavior in a Schottky anomaly ($C/T \sim T^{-3}$). Furthermore, we found the temperature hysteresis phenomenon in specific heat. At 1st run, a sharp anomaly is observed around 1.2 K. Strangely, the anomaly at 1.2 K disappears after repeating the measurement a few times at low temperature. We discuss the upturn below 2 K and the strange sharp peak around 1 K.

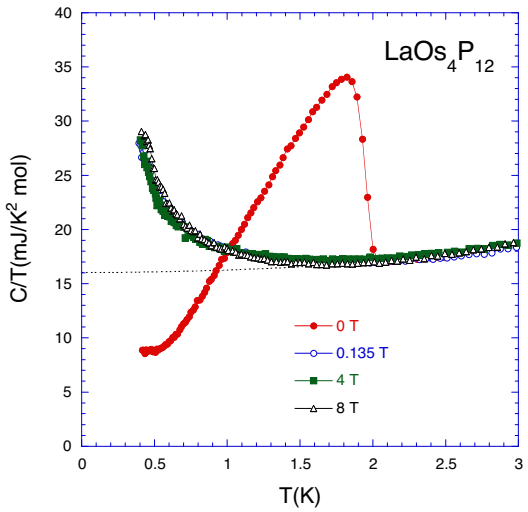

Figure 1: Specific heat divided by temperature C/T of $LaOs_4P_{12}$ at zero field and in the normal state (0.135 T, 4 T and 8 T). The broken line shows the fitting curve by $C/T = \gamma + \beta T^2$; γ=16.2 mJ/K^2 mole and β=3.27×10^{-4} J/K^4 mole.

[1] L.E. DeLong and G. P. Meisner: Solid State Commun. **53**, (1985) 119.

PA05

Electronic structures of Ce-filled skutterudites studied by optical spectroscopy

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Electronic structures of Ce-filled skutterudites $CeRu_4P_{12}$, $CeOs_4P_{12}$, $CeRu_4Sb_{12}$, and $CeOs_4Sb_{12}$ have been studied by means of optical reflectivity experiment at temperatures between 8 and 700 K. The optical conductivity spectra $\sigma(\omega)$ of these compounds have been obtained from the measured reflectivity spectra via the Kramers-Kronig relations. $\sigma(\omega)$ of $CeRu_4P_{12}$ and $CeOs_4P_{12}$ are very similar to those of a narrow gap semiconductor, with an energy gap of $\sim$ 0.2 eV clearly observed even above room temperature. In contrast, $\sigma(\omega)$ of $CeRu_4Sb_{12}$ and $CeOs_4Sb_{12}$ are very similar to those of mixed-valent metals or semiconductors, showing a strongly temperature-dependent energy gap of $\sim$ 10 meV [1]. The electronic structures of these compounds will be discussed based on the present results, and will be compared with those of other experimental techniques and band calculations.

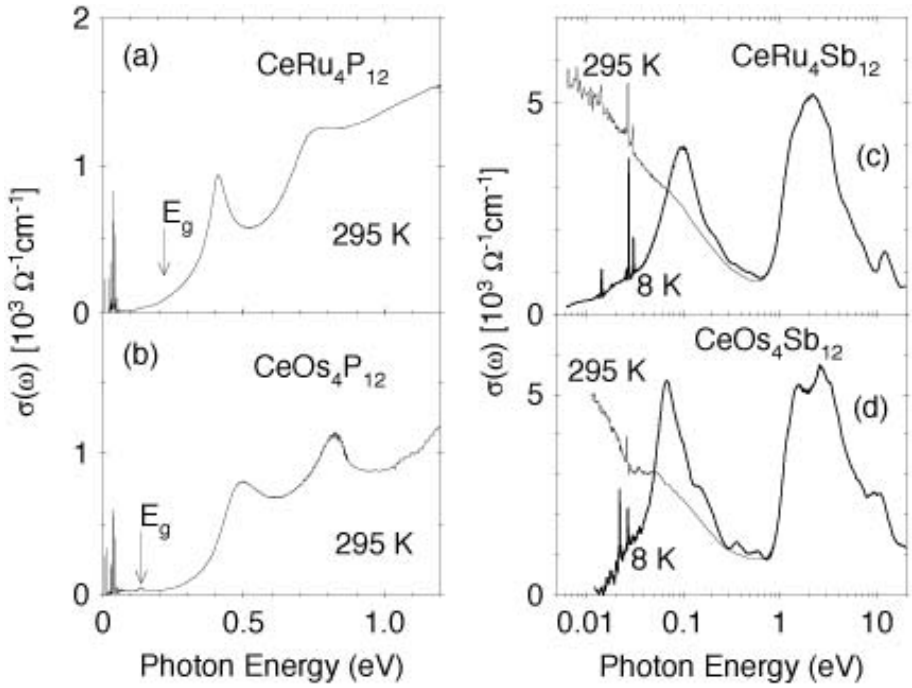

Figure 1: Optical conductivity spectra $\sigma(\omega)$ of four Ce-filled skutterudites. E_g in (a) and (b) indicate the energy gap measured from transport experiments on these compounds.

[1] M. Matsunami, H. Okamura, T. Nanba, H. Sugawara, H. Sato, J. Phy. Soc. Jpn. **72**, (2003) 2722.

PA06

Calculation of Optical Conductivity and Thermoelectric Power of $CeRu_4Sb_{12}$ based on a Realistic Tight-binding Model with Strong Correlation

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abstract

The filled-skutterudite compound $CeRu_4Sb_{12}$ shows a pseudo-gap structure in the optical conductivity spectra similar to the Kondo insulators, but metallic behavior below 80 K[1]. Transport measurements indicate that it would be a semimetal with small overlap of the valence and conduction bands[2,3]. The resistivity shows a large peak at 80 K, and the Seebeck coefficient is positive and also shows a large peak at nearly the same temperature.

In order to explain all these features, we have improved our tight-binding description of the Ce-skutterudite compounds proposed before[4], and constructed a model suitable for the inclusion of the strong correlation together with the specific energy-band features. The model consists of the valence band $\varepsilon^c_{\mathbf{k}} = t_1 \cos\frac{k_x}{2}\cos\frac{k_y}{2}\cos\frac{k_z}{2} + t_2(\cos k_x + \cos k_y + \cos k_z)$ with the nearest and the next-nearest neighbor hoppings on the bcc bravais lattice, which represents the top-most p band of X_{12} clusters, and the f-band $\varepsilon^f_{\mathbf{k}} = \alpha\varepsilon^c_{\mathbf{k}}$. These two bands hybridize with each other through the constant mixing matrix V.

Using this model and introducing the correlation effect within the framework of the dynamical mean field approximation and the iterative perturbation theory, we have successfully calculated the temperature dependences of the optical conductivity, resistivity and the Seebeck coefficient as shown in the Figures below.

We infer that the SDW ordering observed in $CeOs_4Sb_{12}$[5] may be explained by the nesting in the present f-band, and the anomalous field-dependence of the T-B phase boundary[5] may also be explained by our previously proposed theory of spin-fluctuatios[6].

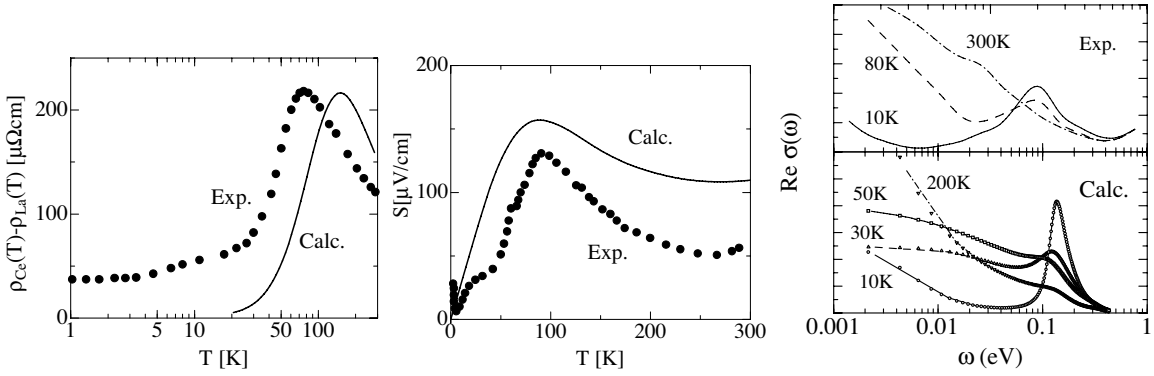

Figure 1: Resistivity, thermopower and optical conductivity calculated for the band model of $CeRu_4Sb_{12}$.

[1] S.V. Dordevic, et al.: Phys. Rev. Lett. **86** (2001)684. [2] N. Takeda and M. Ishikawa, Physica B **259-261** (1999)92. [3] K. Abe, et al, J. Phys.: Condens. Matter **14** (2002) 11757. [4] T. Mutou and T. Saso: J. Phys. Soc. Jpn. 73 No.10 (2004) 2900. [5] H. Sugawara, et al: Phys. Rev. B **71** (2005) 125127. [6] K. Sakurazawa, H. Kontani and T. Saso, J. Phys. Soc. Jpn. **74** (2005) 271.

PA07

Electronic structures of Ce-filled skutterudites investigated by photoemission spectroscopy

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The filled skutterudite compounds with a general formula RT_4X_{12} (R = rare earth; T = Fe, Ru and Os; X = P, As and Sb) have attracted much attention since they exhibit a variety of strongly correlated electron phenomena. Among these compounds, $CeFe_4P_{12}$ is a semiconductor with an energy gap of $\sim$ 130 meV and $CeOs_4Sb_{12}$ shows anomalous temperature dependent transport behavior. These properties suggest a Kondo semiconducting character derived from the hybridization between conduction (c) and Ce f states. In order to clarify the relation between their physical propeties and c-f hybridization, we have investigated the electronic structures of $CeFe_4P_{12}$ and $CeOs_4Sb_{12}$ by the photoemission spectroscopy (PES) using several excitation light sources such as ultrahigh-resolution PES by VUV laser, Ce 3d-4f resonant PES by soft x-ray synchrotron radiation and bulk sensitive core-level PES by hard x-ray synchrotron radiation.

For Ce 3d core-level PES spectra of $CeFe_4P_{12}$, three peak structures due to f^0, f^1 and f^2 final states were clearly observed. With increasing excitation energy from soft x-ray to hard x-ray, a significant enhancement of f^0 and f^2 peak intensity was observed. The result indicates that the c-f hybridization of $CeFe_4P_{12}$ is intrinsically strong. On the other hand, no clear f^0 and f^2 structures were observed for $CeOs_4Sb_{12}$.

We will also discuss the detailed valence band structures of Ce-filled skutterudites from Ce 3d-4f resonant PES and laser-PES spectra. The difference of their spectral properties are qualitatively explained by the degree of c-f hybridization.

PA08

Neutron scattering study of phonon dynamics in a filled skutterudite $CeRu_4Sb_{12}$

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Filled skutterudite compounds RM_4X_{12} (R = rare-earth; M = Fe, Ru or Os; X = P, As or Sb) have attracted great attention due to their potential as thermoelectric devices. In particular, their low lattice thermal conductivity is advantageous to achieve high thermoelectric performance. For further improvement, the origin of their low lattice thermal conductivity needs to be investigated. Previous studies suggest that the suppression of thermal conductivity is a consequence of free vibration of rare-earth atoms in large lattice cages, which is so called rattling effect. To confirm the hypothesis, we have studied phonon behavior of $CeRu_4Sb_{12}$ by neutron scattering using single crystal samples. The measurements were conducted using the 3-axis spectrometers, TAS-1 and TOPAN, at JRR-3M reactor of Japan Atomic Energy Research Institute in Tokai.

Fig. 1 shows energy spectra of transverse acoustic (TA) phonons at various Q positions for CeRu4Sb12 obtained at room temperature. At (6,-0.2,0) near zone-center, a well defined peak is observed. On the other hand, as zone-boundary neared, peak intensity decreases with increasing phonon energy and eventually it vanishes at (6,-0.8,0). Usually, acoustic phonon should be observed clearly also at zone-boundary. The present results suggest that polarization vector of the phonon near zone-boundary vary from that at zone-center. It can be considered that the acoustic mode mixed with optical phonon of which dynamical structure factor is small and located at relatively low energy E 6 or 7 meV. We have identified such low energy optical phonon to be the mode where rare earth atom vibrates largely. The low phonon energy leads to a conclusion that rare-earth atoms bound weakly with surrounded atoms.

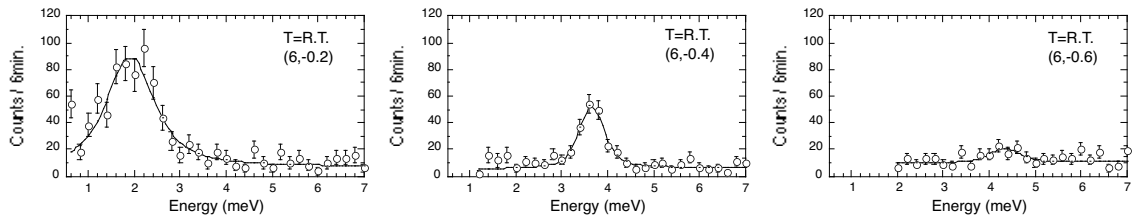

Figure 1: q-dependence of phonon spectrum of $CeRu_4Sb_{12}$ at room temperature.

PA09

Single crystal growth and electric and magnetic properties of $CeFe_4Sb_{12}$

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The filled skutterudite compound $CeFe_4Sb_{12}$ have attracted much attention because of the heavy-fermion behavior and large thermoelectric efficiency [1, 2]. Up till now, poly-crystalline samples have been synthesized and investigated various physical properties. However, there is no report on single-crystalline sample due to its difficulty of synthesize. We have succeeded in growing single crystals for the first time by the Sb-self-flux method and measured the electrical resistivity and magnetization.

Figure 1 shows the temperature dependence of electrical resistivity $\rho(T)$ in $CeFe_4Sb_{12}$. Although the absolute value of resistivity is smaller than those of poly-crystalline samples, the feature of $\rho(T)$ is almost the same with previous reports [2, 3]. $\rho(T)$ shows a weak temperature dependence above $\sim$ 100 K exhibiting a broad minimum at $\sim$ 190 K, and decreases rapidly with decreasing temperature below $\sim$ 100 K. After showing a minimum at $\sim$ 12 K, $\rho(T)$ slightly increases with decreasing temperature and shows saturating tendency at lower temperatures (inset). The behavior above 100 K is a characteristic feature of Kondo effect reflecting CEF[3], however, the origin of increasing in $\rho(T)$ below 12 K is not clear.

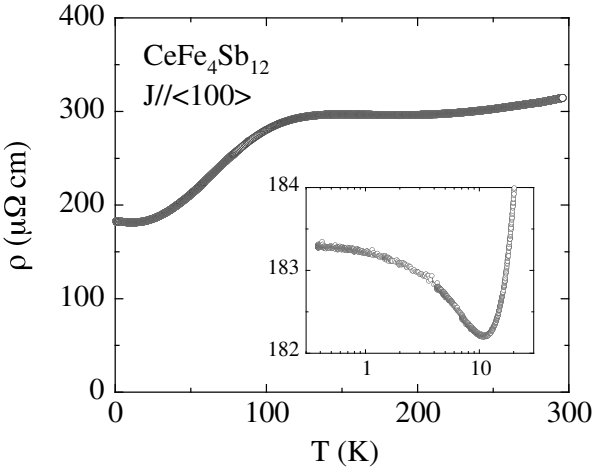

Figure 1: Temperature dependence of the electrical resistivity in $CeFe_4Sb_{12}$.

[1] D.T. Morelli and G.P. Meisner, J. Apple. Phys. **77** (1995) 3777.
[2] D.A. Gajewski et al., J.Phys.Condens Matter **10** (1998) 6973.
[3] R. Viennois et al., J. Magn. Magn. Mater. **272-276** (2004) e113.

PA10

Raman Scattering Study of Filled Skutterudite Compounds

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Raman scattering spectra of filled skutterudite RT_4X_{12}(R=La, Ce, Pr, Nd, Sm : T=Fe, Ru, Os : X=P, Sb) have been measured in order to clarify the lattice dynamical properties. Figure 1 shows Raman spectra of RT_4X_{12} measured at room temperature. Two strong peaks in every spectra are E_g phonons, which are the vibration of pnictogens. Except for the E_g phonons, the crystal field excitation($\bigtriangledown$) in $PrRu_4P_{12}$ and the 2nd-order phonon(▼) in $SmRu_4P_{12}$ and ROs_4Sb_{12} have been observed. These 2nd-order phonons are originated from the excitation of the low energy flat-band in the phonon dispersion curves at the Brillouin zone boundary, which is a characteristic dispersion for the caged crystals. In fact, the first principle calculation shows the existence of the flat band, and the observation of the flat band has been reported by X-ray inelastic scattering. The good energy agreement between the 2nd-order phonons and the twice of the flat-band by the first principle calculation and the X-ray scattering have been obtained. On the other hand, we have not found the similar 2nd-order phonons in RFe_4P_{12}. Then, in order to observe the 2nd-order phonon, the larger cage size than the ionic radius of rare earth ions is necessary. In addition, these peaks vanish at low temperature. The similar results have been already reported for RB_6 crystals[1]. It can be concluded that this temperature dependence of the 2nd-order phonons correlates with the rattling motion of rare-earth ion.

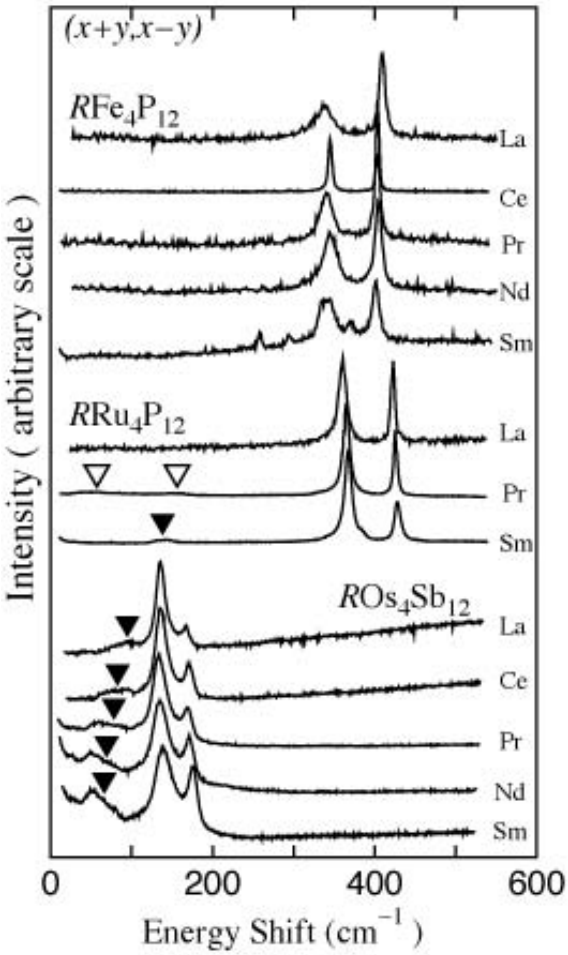

Figure 1: E_g Raman scattering spectra of the filled skutterudite at room temperature.

[1] N. Ogita et al., Phys. Rev. B **68**, (2003) 224605.

PA11

Raman scattering study of guest ion motion in cage crystals

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Recently "rattling" becomes the accepted concept for caged crystals, but its physical property, especially microscopic property, is not well understood. In addition, the relationship between the thermoelectric power and the "rattling" has been pointed out by many research groups. In order to establish the concrete concept of "rattling", the experimental evidences given by dynamical measurements are necessary. We report the results of Raman scattering measurements for the following cage crystals: RB_6 (R=Ca,La,Ce,Pr,Gd,Dy,Yb), RT_4X_{12} (R=rare-earth ion, T=Fe,Ru,Os, X=P,Sb), $X_8Ga_{16}Ge_{30}$ (X = Eu, Sr, Ba), and $La_3Pa_{20}Ge_6$. In the whole experiments, we employed the single crystalline specimens in order to assign the symmetry of the observed peaks, and also measured the temperature dependence between 4K and room temperature. Based on all results, we have found two kinds of the Raman scattering spectra due to the guest ion: 1st or 2nd order Raman scattering processes.

For the trivalent $R^{3+}B_6$ crystals[1], there are 2nd order Raman spectra due to the dispersionless R mode. Their energy and intensity are well determined by the cage size and also their intensity has the clear temperature correlation with the mean square displacement of R ion. However, such temperature dependence has not been observed for the divalent CaB_6 and YbB_6[1]. Thus, the existence of carriers is very important. Similar 2nd order modes has been also observed for metallic RT_4X_{12}(T=Os, X=Sb).

In the clathrate compounds of $X_8Ga_{16}Ge_{30}$, the off-center position of X has been reported by neutron scattering[2]. In fact, we have found the additional peaks in A_g and E_{2g}. Furthermore, at low temperature, the spectra of the guest mode show anomalous spectral change for $Eu_8Ga_{16}Ge_{30}$. We regard that this change is originated from the change of the dynamical properties of the guest Eu ion, that is, from thermal rattling at high temperature to quantum tunneling at low temperature as pointed out by Yotsuhashi et al[3]. In $La_3Pa_{20}Ge_6$, the position La is not off-center, since we have not found the additional peaks.

Finally, we summarize the microscopic properties of "rattling" mode obtained by this study.

1. Flat dispersion phonon mode of guest ion.
2. Energy and intensity determined by the cage size.
3. The existence of the correlation between the intensity and mean square displacement of the guest ion.

[1] N. Ogita et al., Phys. Rev. B **68**, (2003) 224605.
[2] B. C. Sales et al., Phys. Rev. B **63**, (2001) 245113.
[3] S. Yotsuhashi et al, J. Phys. Soc. Jpn. **74**, (2005) 49.

PA12

Rattling and heavy-fermions in the electron-phonon systems with 2nd-order coupling and anharmonic potential

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Recent discovery of rattling motions in the filled skutterdites such as $PrOs_4Sb_{12}$ and the clathrates such as $Ce_3Pd_{20}Ge_6$ has stimulated much interest in strong coupling of local phonons to electrons in heavy-fermion systems[1]. As a simplest realization of such systems, we have investigated the periodic Anderson-Holstein model by using the dynamical mean-field theory combined with the exact diagonalization method[2]. What we have found are; (1) In the strong electron-phonon coupling regime $g \gtrsim g_c$, the system shows an anomalous heavy-fermion behaviour which is accompanied by a large lattice fluctuation and an extreme phonon softening. (2) A simple harmonic potential for $g \lesssim g_c$ changes into an effective double-well potential for $g \gtrsim g_c$. (3) The effective pairing interaction between the conduction electrons has a maximum at $g \approx g_c$.

In the present study, we extend the previous work to include the effects of the 2nd-order electron-phonon coupling g_2 together with the 4th-order anharmonic potential for the ions β. For the strong electron-phonon coupling $g_2 \gtrsim g_{2c}$, the system shows a heavy-fermion behavior with a large mass enhancement factor $m^*/m = Z^{-1}$ together with large charge and lattice fluctuations (Fig.1(a)). With decreasing β, the change becomes steeply in contrast to the case with the 1st-order electron-phonon coupling. We also calculate the effective potential for the ions and find that simple harmonic potential changes into double-well potential in the heavy-fermion regime (Fig.1(b)).

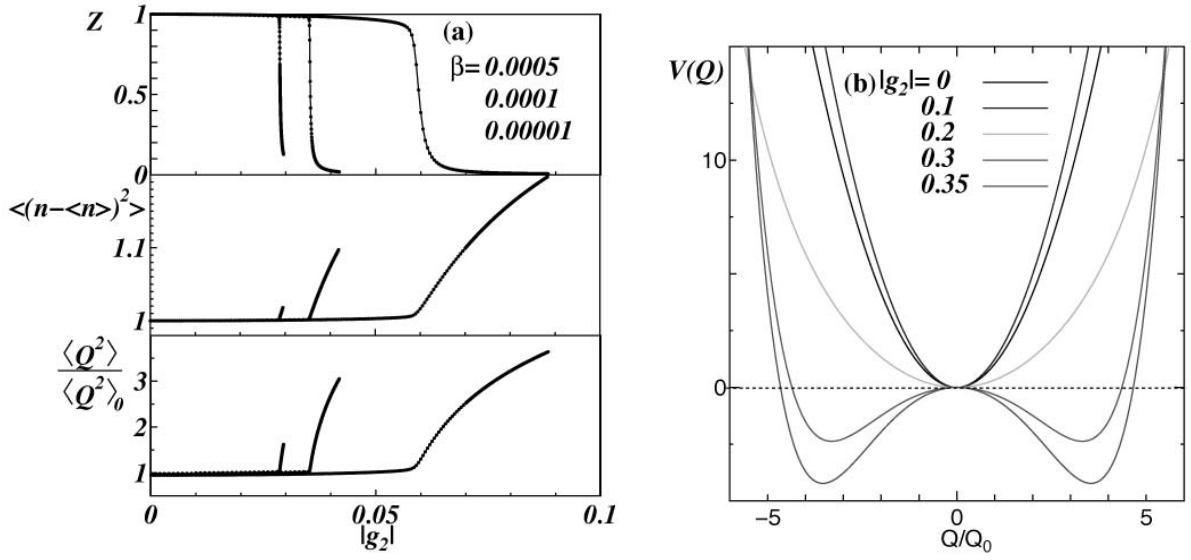

Figure 1: The quasiparticle weight Z, the charge fluctuation $\langle(\hat{n}_i - \langle\hat{n}_i\rangle)^2\rangle$ and the lattice displacement $\langle Q^2\rangle$ as functions of g_2 for several values of β (a). Effective potential for the ions $V_{\rm eff}(Q)$ for several values of g_2 at $\beta = 0.004$ (b).

[1] T. Goto, Y. Nemoto *et al.*,Phys. Rev. B **69** (2004) 180511(R), *ibid* **68** (2003) 184109.
[2] K. Mitsumoto and Y Ōno, Physica C **426-431** (2005) 330.

PA13

La motion in $LaOs_4Sb_{12}$ revealed by ^{139}La-NMR and ^{121}Sb-NQR studies

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The filled skutterudite compounds consist of a large "cage" formed by twelve pnictogen atoms, in which a rare-earth element resides, and show rich variety of ground states depending on the constituent element. One of the topics in the filled skutterudite compounds is that local-vibration modes caused by the rare-earth ion, which is called "rattling", because intimate relationship between unusual heavy-fermion behavior observed in ROs_4Sb_{12} [2,3] and the rattling motion is intensively discussed.

To clarify the nature of the rattling motion from a microscopic point of view, we have performed La-NMR in various La-based skutterudite compounds. Most NMR studies reported so far is on pnictogen atoms such as Sb and P. We consider that the comparison between two NMR results obtained at La and pnictogen atoms can detect additional dynamics observed at the La site, which might be related with the rattling motions.

We have measured the nuclear spin-lattice relaxation rate $1/T_1$ of La and Sb in $LaOs_4Sb_{12}$. The T dependence of $1/T_1$ divided by temperature $1/T_1T$ at the Sb site is scaled with its bulk susceptibility and shows that the dynamics at the Sb site are determined by magnetic fluctuations. On the other hand, $1/T_1T$ at the La site shows a broad peak around 50 K, which is not observed in $1/T_1T$ at the Sb site nor its bulk susceptibility. We consider that the broad peak originates from some non-magnetic mechanism, which is probably ascribed to the rattling motion, because recent ultrasonic measurements found a dispersion in its elastic constant around 50 K in $La(Os_{0.5}Ru_{0.5})_4Sb_{12}$ [4] as in $PrOs_4Sb_{12}$[5].

In our presentation, we will interpret the peak behavior on the basis of a model that the La-rattling motion gives rise to the peak in $1/T_1T$ at the La sites. In addition, we found the La-NMR spectrum broadening below 100 K, which supports this model.

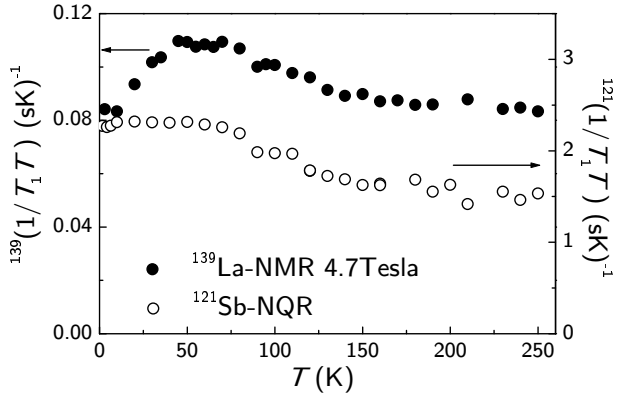

Figure 1: The temperature dependence of $1/T_1T$ at La and Sb sites.

[1] E. D. Bauer *et al.*, Phys. Rev. B **65**, (2002) 100506.
[2] S. Sanada *et al.*, J. Phys. Soc. Jpn **74**, (2005) 246.
[3] T. Yanagisawa *et al.*, private communications.
[4] T. Goto *et al.*, Phys. Rev. B **69**, (2004) 180511(R).

PA14

Rattling in $PrOs_4Sb_{12}$ Studied by Neutron Diffraction

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$PrOs_4Sb_{12}$ was reported to be the first Pr-based heavy fermion superconductor with $T_{sc} = 1.85$ K.[1] The non-magnetic Γ_1 singlet ground state and the existence of field-induced antiferroquadrupolar order phase suggest the important role of quadruploar interaction in forming the Cooper pairs. In addtion, a recent study suggests the importance of 'rattling': the large, localized thermal vibration of Pr under a shallow potential in an over-sized Sb cage.[2] In order to clarify the rattling of Pr ion in $PrOs_4Sb_{12}$, neutron diffraction experiments on powder and single crystalline samples were carried out.[3]

The enormously large thermal mean square displacement of Pr was deduced for room temperature to be $U_{Pr} \sim 0.04$Å^2, roughly corresponding to mean thermal displacement of 0.2 Å. With decreasing temperature, U_{Pr} shows drastic decrease but remains large even at 7.7 K which is twice as large as those of Os and Sb. These results are shown in Fig. 1 The large value of U_{Pr} and its strong temperature dependence indicate the rattling of Pr under the shallow potential in the Sb cage. In order to see the detailed nuclear density distribution, the maximum entropy method (MEM) was employed by using software PRIMA.[4] The obtained nuclear density distribution for room temperature unveils a widely spread Pr distribution in the Sb cage. It is noticeable that the distribution of Pr has a strong anisotropy towards the $\langle 1\,1\,1 \rangle$ direction. This direction corresponds to one of the void of the Sb icosahedron cage.

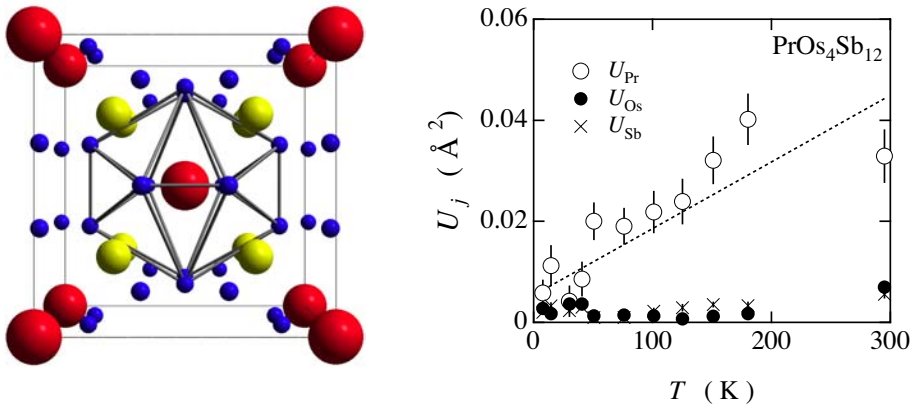

Figure 1: (Left) Crystal structure and (Right) temperature dependence of thermal mean square displacement of $PrOs_4Sb_{12}$

[1] M. B. Maple *et al.*, J. Phys. Soc. Jpn. **71** (2002) Suppl. pp. 23.
[2] T. Goto *et al.*, Phys. Rev. B **69** (2004) 180511(R).
[3] K. Kaneko *et al.*, submitted to J. Phys. Soc. Jpn..
[4] F. Izumi and R. A. Dilanian, "Recent Research Developments in Physics," Vol. **3**, Part II,

PA15

Ultrasonic dispersion resulting from off-center rattling in heavy fermion superconductor $PrOs_4Sb_{12}$

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We have succeeded in the measuring of ultrasonic attenuation coefficient α for a single crystalline sample of $PrOs_4Sb_{12}$. Remarkable ultrasonic dispersion (frequency dependence) has been observed in the elastic constant C_{11} and attenuation coefficient α_{11} related with Γ_{23} symmetry for the longitudinal sound waves propagating along the [100] direction. On the other hand, no dispersion has been found in the elastic constant C_{44} and attenuation coefficient α_{44} with Γ_5 symmetry for the transverse sound waves propagating along [100] with polarization along [010]. The explanation is that ultrasonic dispersion is caused by thermally activated off-center rattling, which has charge fluctuation with Γ_{23} symmetry, of Pr ion inside a Sb cage in $PrOs_4Sb_{12}$. The rattling periodically arrayed in a cage strongly couples to the surrounding conduction electrons. The charge fluctuation of the off-center rattling plays an important role for the appearance of the heavy fermion quasi particle and its superconductivity in $PrOs_4Sb_{12}$.

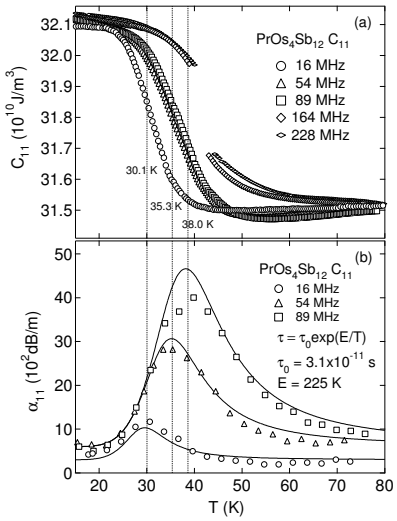

Figure 1: Frequency dependence of the elastic constant C_{11} (a) and attenuation coefficient α_{11} (b). Solid lines in (b) are the fits by Debye-type formula with parameters in the figure.

[1] T. Goto, Y. Nemoto, K. Sakai, T. Yamaguchi, M. Akatsu, T. Yanagisawa, H. Hazama, K. Onuki, H. Sugawara and H. Sato, Phys. Rev. B **69**, (2004) 180511(R).
[2] T. Goto, Y. Nemoto, K. Sakai, K. Onuki, T. Yamaguchi, M. Akatsu, T. Yanagisawa, H. Sugawara and H. Sato, Physica B **359-361**, (2005) 822.
[3] K. Mitsumoto and Y. Ono, Physica C **426-431**, (2005) 330.
[4] S. Yotsuhashi, M. Kojima, H. Kusunose and K. Miyake., J. Phy. Soc. Jpn. **74**, (2005) 49.

PA16

Anomalous superconducting transitions in single crystalline $PrOs_4Sb_{12}$

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After the discovery of superconductivity in $PrOs_4Sb_{12}$ [1], which is to date the only known Pr-based heavy-fermion superconductor, much of experimental evidence have been reported suggesting that the superconductivity is unconventional [2,3]. One of the important aspects is the possible existence of multiphase superconducting (SC) phases suggested from anomalies observed in several physical quantities [4-7].

Specific heat measurements on several samples suggest that the structure around the SC transition exhibits noticeable sample dependence; some samples show apparently double transition structure but others show a jump followed by a lower-temperature kink structure. It does not seem that these structures are indicative of transitions between multiple SC phases. In the constructed magnetic-field-vs-temperature phase diagram, the temperature of the two anomalies ($T_{c1} > T_{c2}$) decreases with increasing magnetic field in a way forming two parallel lines and the magnetic anisotropies of T_{c1} and T_{c2} have the same characteristic behavior. AC magnetic susceptibility for a powered sample shows clear increase in the magnetic shielding around T_{c2}, that is less visible for unpowdered samples. These observations suggest that the double transition structure is rather attributable to the distribution of the superconducting transition temperature in the sample.

Because of the existence of the low-lying crystalline electric field (CEF) excitations of Pr ions, which have been found recently to show significant wave-vector and temperature dependences [8], the precise value of the Sommerfeld electronic specific heat coefficient γ had been difficult to be estimated. However, field dependence data of specific heat allow us to extract thermodynamical character of the heavy-fermion superconductivity to some extent. The results provide evidence for extremely strong-coupling superconductivity in $PrOs_4Sb_{12}$. This feature is discussed in terms of possible sources for the HF superconductivity (excitons or off-center local excitations of Pr ions).

[1] E.D. Bauer *et al.*, Phys. Rev. B **65**, (2002) 100506(R).
[2] H. Kotegawa *et al.*, Phys. Rev. Lett. **90** (2003) 027001.
[3] Y. Aoki *et al.*, Phys. Rev. Lett. **91** (2003) 067003.
[4] R. Vollmer *et al.*, Phys. Rev. Lett. **90** (2003) 057001.
[5] K. Izawa *et al.*, Phys. Rev. Lett. **90** (2003) 117001.
[6] M.-A. Measson *et al.*, Phys. Rev. B **70** (2004) 064516.
[7] T. Cichorek *et al.*, Phys. Rev. Lett. **94** (2005) 107002.
[8] K. Kuwahara *et al.*, Phys. Rev. Lett. **95** (2005) 107003.

PA17

Possible superconducting symmetry in $PrOs_4Sb_{12}$ probed by muon spin rotation

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The discovery of the superconductivity in heavy fermion filled-skutterudite compound $PrOs_4Sb_{12}$ attracted much attention due to the novel properties. $PrOs_4Sb_{12}$ is the first known example of a Pr-based heavy fermion superconductor and exhibits unconventional superconductivity. A field-induced antiferro-quadrupolar ordered phase is laying close to the superconducting phase and therefore, it is argued that quadrupole fluctuations play an important role for the electron paring mechanism in the superconducting phase. One of central issues for this compound is the symmetry of the superconducting order parameter. In our previous precise zero-field μSR in $PrOs_4Sb_{12}$, the weak spontaneous internal magnetic field was observed below superconducting transition temperature. This result provide unambiguous evidence of the time reversal symmetry breaking superconductivity[1]. To clarify the spin state of Cooper pair, we carried out muon spin rotation(μSR) measurements to obtain the Knight shift in $PrOs_4Sb_{12}$.

The experiment was carried out by using single crystalline sample. In the magnetic field which applied to [100] direction, muon Knight shift was clearly observed below 200 K. In the normal phase, Muon Knight shift is temperature dependent and well scaled to bulk susceptibility. At low temperature, no reduction of muon Knight shift passing through T_c is observed. This result is in contrast with a spin-singlet superconductor and suggesting that the spin-triplet SC is realized in $PrOs_4Sb_{12}$[2].

We also carried out the muon Knight shift measurements in $Pr_{1-x}La_xOs_4Sb_{12}$ to elucidate the La substitution effect for the superconductivity. In x=0.4 sample, we obtaine similar results with $PrOs_4Sb_{12}$. The possible superconducting symmetry will be presented.

[1]Y.Aoki et al., Phys. Rev. Lett. 91, 067003(2003).
[2]W.Higemoto et al., submitted.

[1]Present address Department of Physics, McMaster University

PA18

Local magnetization anomaly in $PrOs_4Sb_{12}$ and its spatial distribution

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In this work, superconducting state of $PrOs_4Sb_{12}$ is examined by local magnetization measurements using a micro-Hall probe array. Recently, we have found an anomalous dip in the local magnetization hysteresis near the central magnetization peak, H_{cp}, by a Hall probe with an active area of 30×30 μm^2 (Fig. 1) [1]. The anomaly is characteristic of superconductors with a broken time-reversal symmetry, and is considered to be an evidence for the underlying degenerate chiral domains. Although the dip is considered to be originated from the micro-structure of the superconducting domains, it traces the same curve for every measurement in the same setting, suggesting that the measured signal is an average over a number of domains. To examine the spatial distribution of the local magnetization anomaly, and hence the size of the degenerate domains, local magnetization measurements using an array of Hall probes are performed with each active area of 5×5 μm^2 spaced every 15 μm. Fig. 2 shows the local magnetization hystereses for an active area, P1, of the Hall probe array. The data are less reproducible. They sometimes show a remarkable dip but sometimes not even at the same temperature. Those results suggest that the source of the local magnetization anomaly is spatially inhomogeneous and the scale of the inhomogeneity is comparable to the size of the Hall probes.

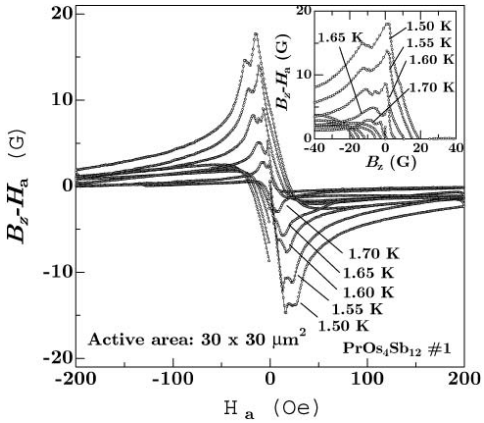

Figure 1: Local magnetization hysteresis curves in $PrOs_4Sb_{12}$ for the [001] axis measured by a Hall probe with an active area of 30×30 μm^2. The inset shows the hysteresis curves as a function of magnetic induction B_z.

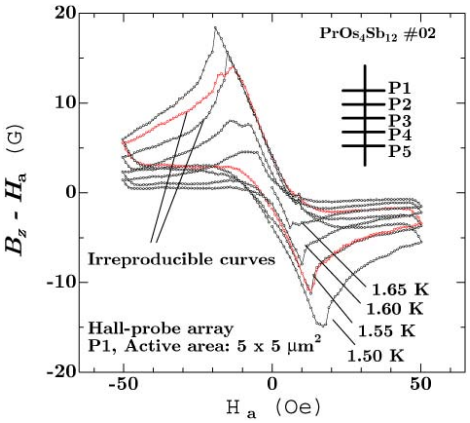

Figure 2: Local magnetization hysteresis curves in $PrOs_4Sb_{12}$ for an active area, P1, of the Hall-probe array. Some data show dip near H_{cp} but some of them do not show it. There appears less reproducibility, and the data traces different curves as in the case of 1.55 K.

[1] S. Kasahara *et al.*, Physica C **426-431**, (2005) 381.

PA19

Pressure effect on magnetic phase diagram of $PrOs_4Sb_{12}$

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The filled skutterudite compound $PrOs_4Sb_{12}$ has attracted considerable attention due to the heavy fermion behavior and unconventional superconductivity (T_c = 1.85 K). In addition to superconductivity, this compound exhibits an antiferroquadrupolar (AFQ) ordering in magnetic fields above 4.5 T. Since the AFQ phase is located close to the superconducting (SC) phase, quadrupolar fluctuations are expected to be responsible for superconductivity of this material. Interestingly, recent inelastic neutron scattering experiments on $PrOs_4Sb_{12}$ revealed the presence of quadrupolar excitons and led to the conclusion that the heavy fermion superconductivity is attributed to the quadrupolar excitons [1]. To further elucidate the relationship between AFQ order and superconductivity in $PrOs_4Sb_{12}$, pressure experiments would be a useful tool. We report the pressure effect on magnetic phase diagram of $PrOs_4Sb_{12}$ studied using DC magnetization measurements.

Figure 1 shows the magnetic phase diagram of $PrOs_4Sb_{12}$ derived from the magnetization measurements. The application of pressure of 1.5 GPa significantly reduces T_c, and the SC phase becomes unstable. Meanwhile, the field-induced AFQ phase shifts to lower fields and approaches to the SC phase. We will discuss the observations in the light of the quadrupolar excitons as origion of superconductivity.

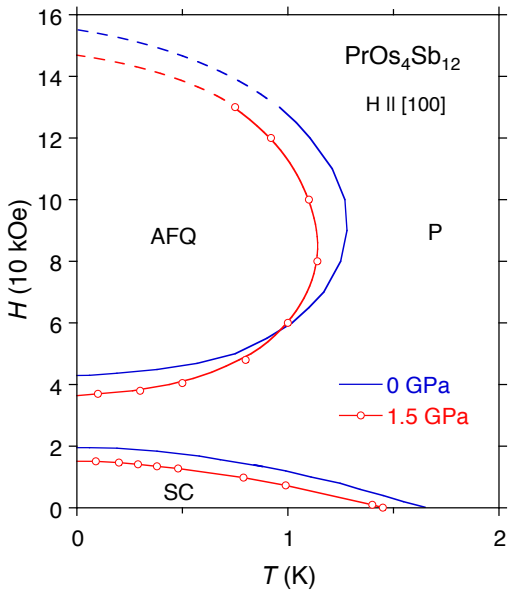

Figure 1: $H-T$ phase diagram for $H \parallel [100]$ in $PrOs_4Sb_{12}$ deduced from magnetization measurements. Blue and red lines represent phase transitions at 0 and 1.5 GPa.

[1] K. Kuwahara *et al.*, Phys. Rev. Lett. **95** (2005) 107003.

PA20

Pressure effect of electrical resistivity and magnetoresistance on $PrOs_4Sb_{12}$

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[2] *National High Magnetic Field Laboratory, Tallahassee, FL 32310-3706, USA*

The filled skutterudite compound $PrOs_4Sb_{12}$ is the first example of a Pr-based heavy fermion superconductor with $T_C \sim 1.85$ K [1]. $PrOs_4Sb_{12}$ has attracted much attention and extensive studies have been being carried out, due to the unusual physical properties of this compound such as unconventional superconductivity and field induced ordered phase. On the other hand, a study of pressure effect on $PrOs_4Sb_{12}$ is hardly reported except for ref.[2] which presents pressure-dependent electrical resistivity up to ~ 2 GPa.

So, to elucidate how the superconductivity does change at $P > 2$ GPa, we have performed electrical resistivity and magnetoresistance measurements on $PrOs_4Sb_{12}$ under high pressure. The measurements of $PrOs_4Sb_{12}$ were carried out by a conventional four-wired method under several pressures up to 8 GPa, temperatures down to 0.3 K and magnetic fields up to 18 T. Piston cylinder pressure cell and newly developed diamond anvil cell were used at $P < 2$ GPa and $2 < P < 8$ GPa, respectively. As shown in Figure 1, superconductivities were observed at all pressures where the measurements have been done. With increasing pressure, T_C decreases under $P < 2$ GPa at a rate $dT_C/dP \sim -0.16$ K/GPa. At $P > 2$ GPa, pressure effect on T_C became to be smaller and a value of T_C be saturated to constant ~ 1.4 K above 4 GPa as indicated in Figure 2. The results of measurements including a phase diagram under high field will be discussed in detail. In addition, detail of newly developed diamond anvil will be also reported.

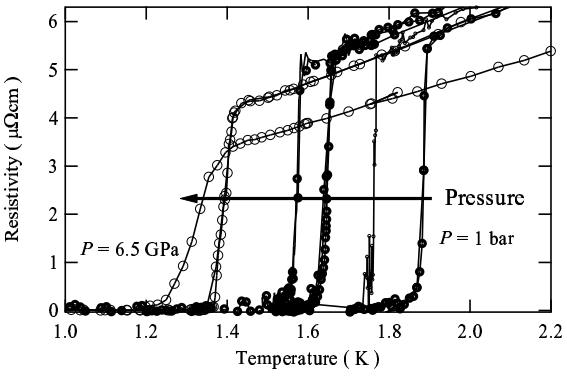

Figure 1: Electrical resistivities of $PrOs_4Sb_{12}$ as a function of temperature under several pressures.

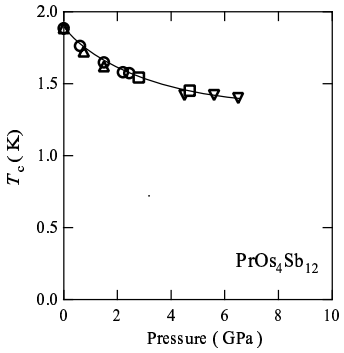

Figure 2: Pressure dependence of T_C.

[1] E. D. Bauer et al.: Phys. Rev. B 65, (2002) 100506.
[2] M. B. Maple et al.:J. Phys. Soc. Jpn. 71, (2002) Suppl. pp. 23.

PA21

Neutron scattering study on low energy excitations of the Heavy-Fermion Superconductor $PrOs_4Sb_{12}$

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We report inelastic neutron scattering experiments performed to investigate the low energy magnetic excitations of single crystals of the first Pr-based heavy-fermion superconductor $PrOs_4Sb_{12}$ [1]. In both superconducting and normal states, the observed excitation clearly softens at a wave vector $Q = (1,0,0)$, which is the same as the modulation vector of the field-induced antiferro-quadrupolar ordering and its intensity at $Q = (1,0,0)$ is smaller than that around zone center, as shown in Fig. 1. This result directly evidences that this excitonic behavior is derived mainly by a nonmagnetic quadrupolar interaction between 4f electrons. Furthermore the tendency of narrowing of linewidths of excitations below the superconducting transition temperature may suggest that the new 'quadrupolar' excitons are coupled to the heavy-fermion superconductivity.

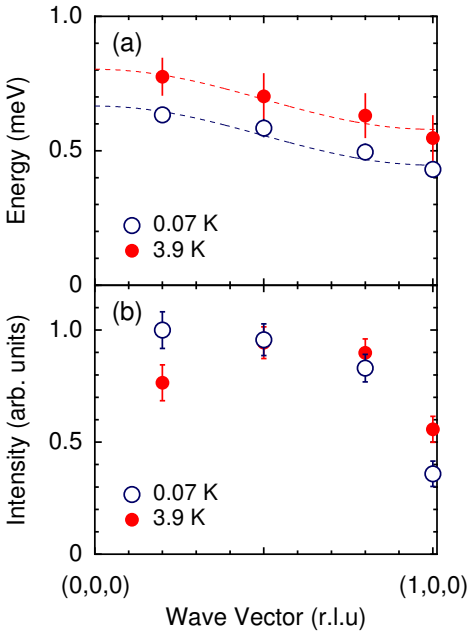

Figure 1: (a) Dispersion relations for the low energy magnetic excitations and (b) Q-dependence of the integrated intensity along the [1, 0, 0] direction at 0.07 K (open circle) and 3.9 K (closed circle). Dashed lines are guides for the eyes.

[1] K. Kuwahara *et al.*, Phys. Rev. Lett. **95**, 107003 (2005).

PA22

Superconducting properties of $(Pr_xLa_{1-x})Os_4Sb_{12}$

Yuki. Yonezawa[1], Yuji. Aoki[1],Yoshino. Tunashima[1], Syotaro. Sanada[1], Daisuke. Kikuchi[1], H. Sugawara[2] and Hideyuki. Sato[1]

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The filled skutterudite $PrOs_4Sb_{12}$ has been reported the shown an unconventional superconductivity which have the possibility of multiple superconducting phases, point nodes. As possible origins, exitons and rattling have been pointed out. In order to investigate the relation between the unconventional superconductivity and those degrees of freedom, study on La-substitution effects on the superconductivity is useful. Using high quality single crystals, we have studied superconducting properties of the series of $(Pr_xLa_{1-x})Os_4Sb_{12}$ by measurements of specific heat C(T) and magnetic susceptibility χ (T).

Figure 1 shows the concentration (x) dependence of T_C determined by the jump in C(T), which is consistent with the reported results[1]. The continuous decrease in T_C is quite different from the existence of a minimum in $Pr(Os_{1-y}Ru_y)_4Sb_{12}$ [2]. The obtained superconducting phase diagram is shown in Fig 2. Contrary to T_C, the value of the upper critical field H_{C2} decreases quickly in the low La-concentration region. This fact suggests that the effective mass of quasiparticles depends sensitively on the Pr concentration.

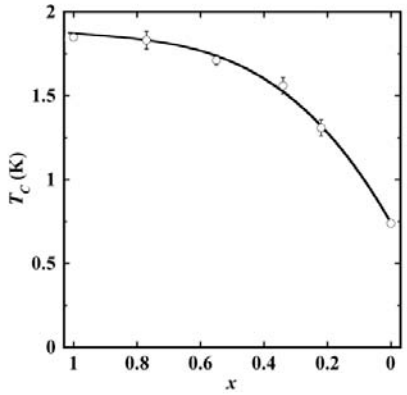

Figure 1: T_C as a function of La concentration x.

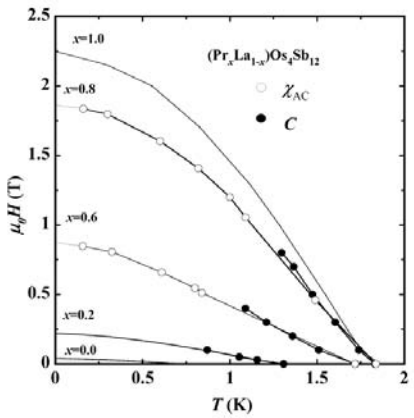

Figure 2: H-T phase diagram of $(Pr_xLa_{1-x})Os_4Sb_{12}$

[1] C. R. Rotundu et al. cond-mat/0402599

[2] N. A. Frederick et al. Phys Rev. B. **69** (2004) 024523.

PA23

Superconducting Characteristics on $(Pr_{1-x}La_x)Os_4Sb_{12}$: ^{121,123}Sb-NQR Study

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We report on superconducting (SC) characteristics for $(Pr_{1-x}La_x)Os_4Sb_{12}$ (x = 0.05, 0.2, 0.4, 0.8) via the measurement of nuclear spin-lattice relaxation rate $1/T_1$. Our previous work has revealed that the $1/T_1$ in $PrOs_4Sb_{12}$ shows neither a coherence peak just below T_c = 1.85 K nor a T^3 like behavior that used to be observed for unconventional heavy-fermion (HF) superconductors with the line-node gap [1]. To clarify the role of Pr^{+3} derived $4f^2$-electrons, we carried out Sb-NQR study on $(Pr_{1-x}La_x)Os_4Sb_{12}$.

Previously reported $1/T_1$ for the La-substitution samples exhibit no coherence peak just below T_c up to La-20 % doping and looks like a $T_1T = const$ behavior far below T_c irrespective of La content as shown in Fig.1. This result suggests that the non-magnetic La impurities induce the residual density of states at the Fermi level as observed for the unconventional superconductors with the nodes in the SC gap function, whereas T_c does not decrease at all up to 20 % - La doping which break up a coherency for $4f^2$ electrons derived HF state. It seems, therefore, that a band responsible for an anisotropic SC energy gap does not play any primary role for the onset of superconductivity in $PrOs_4Sb_{12}$. This unusual impurity effect implies that the local interaction between f^2 electrons and conduction ones plays a key role for the unconventional superconductivity in $PrOs_4Sb_{12}$. Figure 1 also shows the temperature (T) dependencies of $1/T_1$ for x = 0.8 sample. This sample shows the clear coherence peak below T_c which points to the onset of the fully gapped s-wave SC. Here, an interesting point is that $T_c \sim$ 1.05 K of this sample is higher than T_c = 0.74 K for $LaOs_4Sb_{12}$ and yet the onset temperature T_{on} = 1.34 K below which SC diamagnetism appears is higher than $T_c \sim$ 1.04 K. From these results, it is remarked that the Pr substitution for La increases T_c, and causes SC fluctuations which emerges below the onset temperature. This unusual SC behaviors observed by the Pr substitution for La may give an hint for understanding the unconventional SC mechanism for $PrOs_4Sb_{12}$.

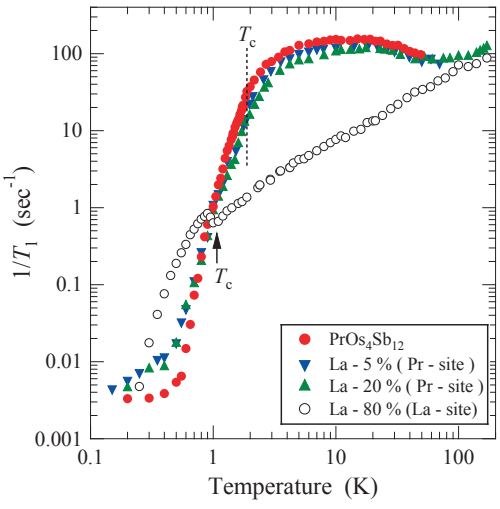

Figure 1: Temperature dependence of $1/T_1$ for $(Pr_{1-x}La_x)Os_4Sb_{12}$.

[1] H. Kotegawa, M. Yogi, Y. Imamura, Y. Kawasaki, G. -q. Zheng, Y. Kitaoka, S. Ohsaki, H. Sugawara, Y. Aoki, and H. Sato, Phys. Rev. Lett. **90** (2003) 027001.

PA24

Impurity as a smoking gun for the superconducting gap symmetry of Skutterdite heavy fermion compound $PrOs_4Sb_{12}$

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In order to get a clue on the superconducting gap symmetry of the Skutterdite heavy fermion compound $PrOs_4Sb_{12}$, we replace part of Os with Ru and study the change in the superconducting property using NQR technique. We performed NQR experiments using the sample $Pr(Os_{1-x}Ru_x)_4Sb_{12}$ $[x = 0.1, 0.2]$. The temperature dependence of the relaxation rate are shown in Fig. 1 and shows T_1T= constant in the low temperature region ,$T<T_c$. We find that the impurity brings about a finite density of states at the Fermi level, which suggests the presence of nodes in the gap function [1]. We will present detailed data for various Ru contents and compare our results with theory.

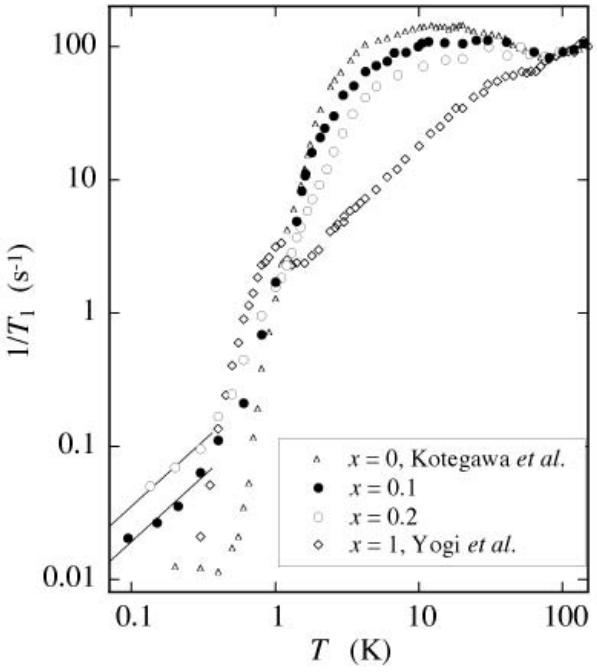

Figure 1: Temperature dependence of $1/T_1^S$ in $Pr(Os_{1-x}Ru_x)_4Sb_{12}$ $(x = 0.1, 0.2)$. Data for $PrOs_4Sb_{12}$ [2] and $PrRu_4Sb_{12}$ which is a BCS superconductor [3] are also shown for comparison. The straight lines indicate the T_1T=const relations.

[1] M. Nishiyama, *et al.*, J. Phys. Soc. Jpn. **74** (2005) 1938.
[2] H. Kotegawa, *et al.*, Phys. Rev. Lett. **90** (2003) 027001.
[3] M. Yogi, *et al.*, Phys. Rev. **B 67**, (2003) 180501(R).

PA25

Specific Heat of $La(Os_{1-x}Ru_x)_4Sb_{12}$

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In contrast to the usual BCS-type superconductor $PrRu_4Sb_{12}$, a superconducting state of $PrOs_4Sb_{12}$ is very unconventional. It is reported that the superconducting transition temperature of mixed crystals $Pr(Os_{1-x}Ru_x)_4Sb_{12}$ exhibits a minimum at around x=0.6 where competition of two types of superconductivity is suggested[1]. We also found the change of crystalline field at almost the same point x=0.6. On the other hand, the off-center rattling motion of a Pr ion in a Sb-cage is a characteristic of $PrOs_4Sb_{12}$[2] and its relevance to the unconventional superconductivity is suggested, because there in no report of the rattling motion in $PrRu_4Sb_{12}$. To clarify the relation between the rattling motion and the Ru-content, we measured specific heat of $La(Os_{1-x}Ru_x)_4Sb_{12}$. To evaluate the contribution of the La ion to the specific heat, we subtracted the specific heat of $RhSb_3$ from that of $La(Os_{1-x}Ru_x)_4Sb_{12}$ and the results are shown in figure 1. A broad peak of the specific heat around 80 K is observed for all x value, and this peak is enhanced with decreasing Ru-content. The relationship between this anomaly of the specific heat and the rattling motion of the La ion will be discussed.

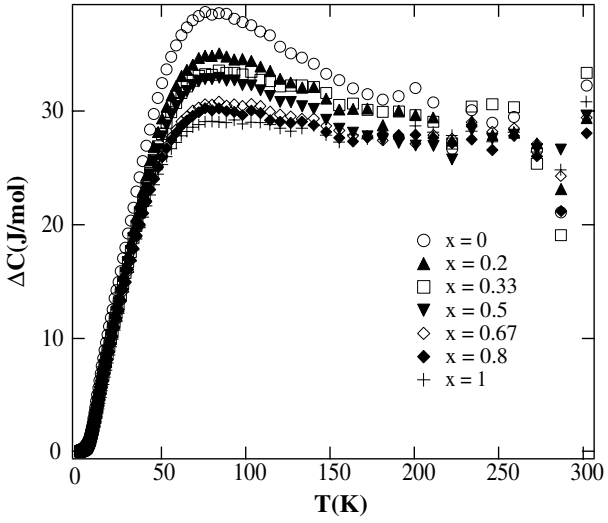

Figure 1: Contribution of the La ion to the specific heat in $La(Os_{1-x}Ru_x)_4Sb_{12}$, which is obtained by subtracting the specific heat of $RhSb_3$ from that of $La(Os_{1-x}Ru_x)_4Sb_{12}$. A broad peak at about 80K becomes large with decreasing Ru-content x.

[1] N. A. Frederick, T. D. Do, P. -C. Ho, N. P. Buch, V. S. Zapf and M. B. Maple, Phys. Rev. B **69**, (2004) 024523.

[2] T. Goto, Y. Nemoto, K. Sakai, T. Yamaguchi, M. Akatsu, T. Yanagisawa, H. Hazama, K. Onuki, H. Sugawara and H. Sato , Phys. Rev. B **69**, (2004) 180511.

PA26

Roles of Multipoles and Excitons in Superconductor $PrOs_4Sb_{12}$

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abstract

The variety of physics in the filled skutterudite compounds is realized by changing the combination of RT_4X_{12} (R is a rare-earth or U; T is one of transition metals: Fe, Ru or Os; X is a pnictogen: P, As or Sb). The rich physics is expected to be understandable by a simple model containing a few parameters such as crystal-field parameters for rare-earth ions and exchange couplings of the f-electron states with conduction electrons. Among them we focus on $PrOs_4Sb_{12}$ that is the first superconductor of Pr-based metallic compounds. In the present study, we discuss a possibility of exciton-mediated mechanism as an origin of this superconductivity [1].

In this compound the low-lying crystal-field states of Pr form a pseudo-quartet consisting of Γ_1 singlet ground and $\Gamma_4^{(2)}$ triplet excited states. The dispersive crystal-field excitations (excitons) have been detected experimentally. Considering both magnetic and nonmagnetic couplings of conduction electrons with the pseudo-quartet, we determine the effective interaction between conduction electrons and the pseudo-quartet states. The nature of exchange processes is related closely to a_u and t_u components of the conduction electrons that correspond to the molecular orbitals of an Sb_{12} cage surrounding a Pr ion. By the second-order perturbation in the exchange coupling, Cooper pairing interactions are derived both for singlet and triplet superconductivities.

We find that the T_h symmetry, which is a unique feature of the filled skutterudite compounds, plays an important role in realizing a triplet superconducting state. As a candidate for the superconductivity in $PrOs_4Sb_{12}$, we propose a nonunitary triplet state (e.g., $\Gamma_{4x} + i\Gamma_{4y}$) with twofold symmetry which agrees most naturally with the gap structure observed in the low field phase. We also discuss anisotropy of spin susceptibility reflecting the T_h symmetry of gap functions to give useful information to Knight-shift measurements (see Table 1).

Table 1: Possible types of gap functions under the T_h symmetry ($\omega = e^{\pm i2\pi/3}$).

pairing state	gap function	spin susceptibility
(a) Γ_1	T_h	$\chi_{xx} = \chi_{yy} = \chi_{zz}$
(b) $\Gamma_{23,\mathrm{I}},\ \Gamma_{23,\mathrm{II}}$	D_{2h}	$\chi_{xx} \neq \chi_{yy} \neq \chi_{zz}$
(c) $\Gamma_{23,\mathrm{I}} \pm i\Gamma_{23,\mathrm{II}}$	T_h	$\chi_{xx} = \chi_{yy} = \chi_{zz}$
(d) $\Gamma_{4x},\ \Gamma_{4y}\ , \Gamma_{4z}$	D_{2h}	$\chi_{xx} \neq \chi_{yy} \neq \chi_{zz}$
(e) $\Gamma_{4y} \pm i\Gamma_{4z},\ \Gamma_{4z} \pm i\Gamma_{4x},\ \Gamma_{4x} \pm i\Gamma_{4y}$	D_{2h}	$\chi_{xx} \neq \chi_{yy} \neq \chi_{zz}$
(f) $\Gamma_{4x} \pm \Gamma_{4y}\ \pm \Gamma_{4z}$ (fourfold degeneracy)	D_{3d}	$\chi_{xx} = \chi_{yy} = \chi_{zz}$
(g) $\Gamma_{4x} \pm \omega\Gamma_{4y}\ \pm \omega^2\Gamma_{4z}$ (eightfold degeneracy)	D_{3d}	$\chi_{xx} = \chi_{yy} = \chi_{zz}$

[1] M. Matsumoto and M. Koga, J. Phy. Soc. Jpn. **73**, (2004) 1135; *ibid.* **74**, (2005) 1686.

PA27

Estimation of pf-hybridization in Pr skutterudites by using the LMTO band calculation

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The filled skutterudite $PrFe_4P_{12}$ shows the Kondo like behavior in the electrical resistivity [1] and in the NMR experiment [2]. The resonant photoemission spectrum (RPES) of f-electrons in Pr-skutterudites shows a three-peak structure [3]. In $PrFe_4P_{12}$ the intensity just below the Fermi level is very large in comparison with other Pr-skutterudites such as $PrRu_4P_{12}$ and $PrRu_4Sb_{12}$. We have calculated the RPES of $PrFe_4P_{12}$ by using the non-crossing approximation for the impurity Anderson model [4]. The large intensity can be explained by the combination of Kondo resonance and its satellites which are formed in terms of many f^2 multiplets that accompany a hole in the valence band.

In this paper we estimate the hybridization intensity for various Pr-skutterudites in the following way in order to discuss the difference of intensity of resonance peak of RPES of Pr-skutterudites. It is assumed that the hybridizations for PrT_4X_{12} and LaT_4X_{12} are comparable. The hybridization intensity is given as $W_\Gamma(\varepsilon) = \mathrm{Im}\{G_\Gamma(\varepsilon)^{-1} - \varepsilon + \epsilon_f\}/\pi$, where $-\mathrm{Im}G_\Gamma(\varepsilon)/\pi$ is the non-interacting partial density of states (PDOS) of f-electron of La in LaT_4X_{12}. The PDOS of LaT_4X_{12} is calculated by employing the LMTO method. In Fig. 1 we show the hybridization intensity for $LaFe_4P_{12}$, $LaRu_4P_{12}$ and $LaOs_4Sb_{12}$. The hybridization intensity for $LaFe_4P_{12}$ is lager than that for $LaRu_4P_{12}$. This is a possible scenario that the resonance peak of RPES for $LaFe_4P_{12}$ is lager than that for $LaRu_4P_{12}$.

In $LaOs_4Sb_{12}$ the hybridization intensities with Γ_7 and Γ_8 symmetries at the Fermi level are about the same. We will discuss the heavy fermion behavior of $PrOs_4Sb_{12}$ [5].

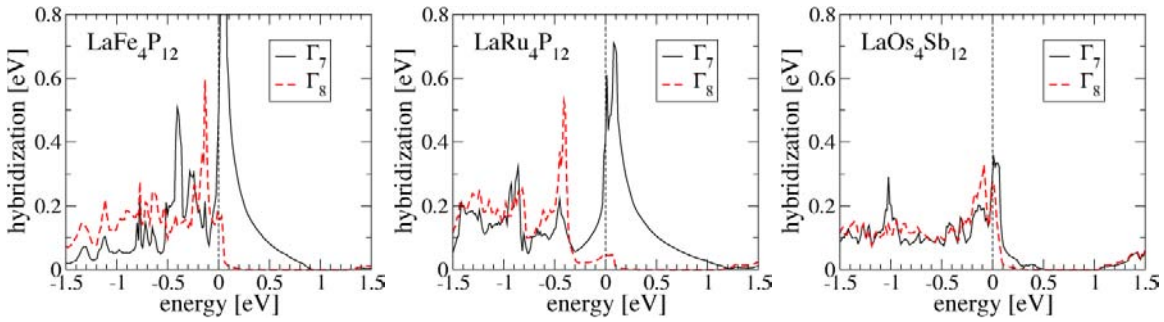

Figure 1: The calculated hybridization intensity for various La skutterudites. The solid (dashed) line shows the hybridization with Γ_7 (Γ_8) symmetry of the point group O_h. The Fermi level is an origin of the energy.

[1] H. Sato et al, Phys. Rev. B. **62** (2000) 15125.
[2] K. Ishida et al, Phys. Rev. B. **71** (2005) 24424.
[3] A. Yamasaki et al, Phys. Rev. B. **70** (2004) 113103.
[4] Y. Shimizu et al, proceedings of SCES'05.
[5] Y. Shimizu and O. Sakai, J. Phys. Soc. Jpn. **74**, (2005) 27.

PA28

Valence Fluctuation from f^2 Singlet Crystal-Field Ground State in Generalized Periodic Anderson Model

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The relevant degrees of freedom in some Pr- and U-based compounds at low temperature are believed to be two almost-localized electrons on atomic f orbitals. The properties of such f^2 systems have been a long-standing issue in heavy-fermion physics over the last two decades. Recently, a new class of cubic Pr compounds, called skutterudites, has attracted much attention due to variety of unusual low-temperature phenomena [1][2]. It has been revealed experimentally that among crystal-field (CF) multiplets in the f^2 configuration, a singlet ground state is often realized in this class of materials.

Generally, hybridization of f states with conduction bands is believed to be the origin of the heavy-fermion anomaly. Therefore, the recent experimental findings on skutterudites pose a well-defined question regarding the nature of hybridization and the resulting valence fluctuation in such f^2 singlet systems. As a first step to attack this problem, we study here a generalized periodic Anderson model (PAM) with an f^2 singlet-triplet CF level scheme. We particularly address whether and how two f electrons approach the singlet localized state as a function of CF splitting.

In this study, we formulate a Gutzwiller-type variational method (GM) for a two-orbital PAM that corresponds to a realistic Γ_8 model. In the GM [3], occupation probabilities of local many-body states are determined variationally so as to balance hybridization and Coulomb interaction. We show that the ratio of the singlet to triplet occupations is closely related to valence fluctuation from the f^2 configuration. As a result, valence fluctuation undergoes marked suppression as the splitting increases. The GM predicts that this valence change is discontinuous in the case of small hybridization. Since the occupation suddenly becomes close to f^2 at the critical strength of CF, it can be regarded as a localization-delocalization transition. The influence of the CF scheme on magnetic properties is studied in terms of the Landau parameter of magnetic susceptibility. It is shown that the CF splitting changes the characteristics of the quasi-particle interaction, resulting in a strong suppression of susceptibility. A part of this work will be published in ref. [4].

[1] Y. Aoki *et al.*, J. Phys. Soc. Jpn. **74**, (2005) 209.

[2] Some properties of the singlet-triplet crystal field model for skutterudites are discussed in R. Shiina, J. Phys. Soc. Jpn. **73**, (2004) 2257.

[3] J. Bünemann *et al.*, Phys. Rev. B **10**, (1998) 6896.

[4] R. Shiina, J. Phys. Soc. Jpn. **74**, (2005) No.12.

PA29

Valence Fluctuations in an Extended Periodic Anderson Model

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Usually, superconductivity in heavy fermion (HF) compounds is believed to be caused by enhanced antiferromagnetic (AF) spin fluctuations. In $CeCu_2Si_2$ and in some of the so-called Ce-115 componds, however, it seems difficult to ascribe the occurrence of superconductivity to the AF spin fluctuations alone. The superconducting transition temperature varies nonmonotonically as the system is driven away from the AF quantum critical point by, for example, pressure.

Onishi and Miyake argued that the enhanced valence fluctuations might cause superconductivity in those compounds, and indeed found that the valence fluctuations were considerably enhanced by the repulsive interaction U_{cf} between a conduction electron and an f-electron, which caused d-wave superconductivity [1]. Recently, Watanabe also found the enhancement of the valence fluctuations and valence instability critical point in a 1D extended periodic Anderson model using the density matrix renormalization group method [2].

We study the extended periodic Anderson model, the same model as those studied in [1,2], using the dynamical mean field theory and the fluctuation-exchange approximation. We have found that the valence fluctuations are indeed enhanced by U_{cf} with the dynamical mean field theory in agreement with the previous studies. We extend the study to more strongly correlated region and to lower temperatures, and also study the possible superconductivity caused by the enhanced charge fluctuations.

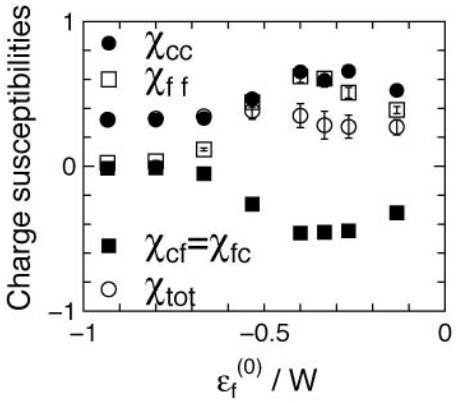

Figure 1: The uniform charge susceptibility (open dots), $\chi^{\rm c}_{cc}$ (solid dots), $\chi^{\rm c}_{cf} = \chi^{\rm c}_{fc}$ (solid squares) and $\chi^{\rm c}_{ff}$ (open squares) as functions of the f-electron level ϵ_f. The Coulomb interaction between f-electrons $U = 6$, $U_{cf} = 2$, the conduction band width $2W = 6$, the mixing $V = 0.4$, and the total electron number $n_{\rm tot} = 1.75$

[1] H. Onishi and K. Miyake, J. Phys. Soc. Jpn. **69** (2000) 3955; Physica **281** & **282** (2000) 191.
[2] S. Watanabe, private communications.

PA30

Theory of Transport Phenomena in 3D Strongly Correlated Systems Close to a Magnetic Quantum-Critical Point

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[2]*Department of Physics, Nagoya University, Nagoya 464-8602, Japan*

Recently, heavy fermion metals close to antiferromagnetic (AF) quantum critical points (QCP) have attracted much attention. Various transport coefficients in these compounds, like $CeCoIn_5$, $CeCu_{5.9}Au_{0.1}$ and $YbRh_2Si_2$, show striking non-Fermi liquid-like behaviors. In $CeCoIn_5$, for example, the resistivity ρ is T-linear below $T_{\rm coh} \sim 20$K. The Hall coefficient $R_{\rm H}$ takes a small constant value ($\sim -3 \times 10^{-10} m^3/C$) above 40K, whereas its absolute value increases in proportion to T^{-1} below $T_{\rm coh}$; $R_{\rm H} \approx -6 \times 10^{-9} m^3/C$ just above $T_{\rm c} = 2.3$K. That is, $|R_{\rm H}(2.5K)|/|R_{\rm H}(100K)|$ reaches to 20. In the same way, the Nernst coefficient ν takes an extremely huge value ($\sim -1\mu V/KT$) just above $T_{\rm c}$. These striking non-Fermi liquid-like behaviors cannot be explained in terms of the relaxation time approximation (RTA).

Here, we study a 3D Hubbard model based on the FLEX approximation. The dispersion of an electron is $\epsilon_k = 2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y + 2t''(\cos 2k_x + \cos 2k_y) + 2t_z \cos(k_z)$; we put $(t, t', t'') = (-1, 1/6, -1/5)$ which corresponds to a hole-doped high-$T_{\rm c}$ cuprates. We introduce the the three-dimensionality by t_z. Figure 1 shows ρ, $R_{\rm H}$ and ν for $t_z = 0 \sim 0.8$. The current vertex correction (CVC) is taken into account to satisfy the conservation law, which is totally dropped within the RTA. We find that, even in 3D systems, $R_{\rm H}$ is strongly enhanced nearby the AF QCP due to the CVC. In contrast, $R_{\rm H}$ by the RTA decreases as T does. In conclusion, the CVC is indispensable to understand anomalous transport phenomena in 3D heavy fermion metals close to the AF QCP.

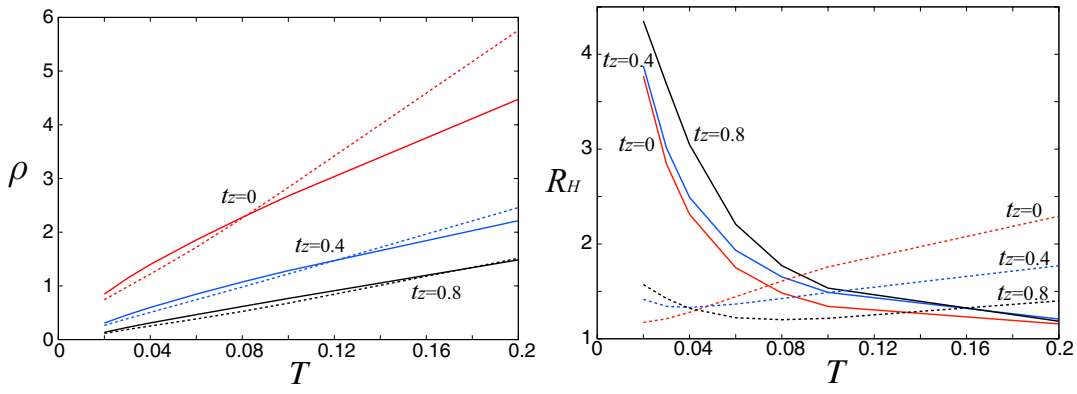

Figure 1: Temperature dependence of ρ and $R_{\rm H}$ given by the CVC-FLEX approximation (full line) and the RTA (broken line). The value of U is 8, 6.3, 5.7 for $t_z = 0, 0.4, 0.8$, respectively. The Stoner factor at $T = 0.02$ is 0.995 in each case, which means that the "distance" from the QCP is same.

[1] Y. Nakajima, K. Izawa, Y. Matsuda, S. Uji, T. Terashima, H. Shishido, R. Settai, Y. Onuki and H. Kontani: J. Phy. Soc. Jpn. **73** (2004) 5.
[2] H. Kontani, K. Kanki, and K. Ueda: Phys. Rev. B **59** (1999) 14723.

PA31

Fermi surface study of heavy fermion system $CeRu_2Si_2$ by LDA+U method

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$CeRu_2Si_2$ is known as a typical heavy fermion system with the nonmagnetic ground state. This material crystalizes in a tetragonal $ThCr_2Si_2$-type structure (Space group I4/mmm) and undergoes metamagnetic transition at the magnetic field of $H_M \sim$ 7.7 T applied along the *c*-axis. The metamagnetic transition has been studied by using various experimental methods, then recognized as crossover transition.

Band structure calculations have been performed for the paramagnetic state of $CeRu_2Si_2$ [1] and $LaRu_2Si_2$ [2] based on the local density approximation(LDA). Although the calculated Fermi surfaces (FS) explain experimental dHvA frequencies qualitatively, the accuracy is not so excellent and cannot identify some experimental dHvA frequencies. In addittion, it is considered that the Ce 4f-electrons, which have itinerant property in the paramagnetic phase, become localized after the metamagnetic transition because the dHvA frequencies for $LaRu_2Si_2$ is similar to those for $CeRu_2Si_2$ in the higher magnetic field region $H>H_M$. However the electronic structure of $CeRu_2Si_2$ is not known well after the metamagnetic transition. Therefore the theoretical electronic structure study in the magnetic field is desired.

We applied an FLAPW-LDA+U method to $CeRu_2Si_2$ and an FLAPW-LDA method to $LaRu_2Si_2$. We have carried out the calculation with various Wyckoff position parameters of Si site because it is not determined experimentally. We have calculated the total energy of $LaRu_2Si_2$ and determine the Wyckoff position from the total energy minimum. We found that in $CeRu_2Si_2$ some dHvA frequencies are very sensitive to the position of Si. In the LDA+U method, some occupied 4f statets are chosen for the initial density matrix because it is not known experimentally, and then determined selfconsistently. It is found that some Fermi surfaces are quite different from experimental results for the initial occupired 4f states as $j_z=\pm 1/2$ Kramers pair. Moreover, we have extended our method to calculate magnetic states including the spin-orbit interaction. We will discuss the electronic structure of $CeRu_2Si_2$ under magnetic field, based on the calculated results.

[1] E. K. R. Runge, R. C. Albers, N. E. Christensen and G. E. Zwicknagl, Phys. Rev. B **51**(1995)10375. H. Yamagami and A. Hasegawa, J. Phys. Soc. Jpn. **62**(1993)592.
[2] H. Yamagami and A. Hasegawa, J. Phys. Soc. Jpn. **61**(1992)2388.

PA32

Change of the Fermi surface in $CeIn_3$ from localized to itinerant across the critical pressure

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$CeIn_3$ with the $AuCu_3$-type cubic crystal structure is a well known Kondo-lattice compound with antiferromagnetic ordering at $T_N = 10\,K$. With increasing pressure, the Néel temperature decreases and becomes zero around a critical pressure $P_c \simeq 2.5\,GPa$ in which the narrow pressure region superconductivity appears below T_{sc}=0.2 K [1].

The Fermi surface of $CeIn_3$ at ambient pressure is similar to that of $LaIn_3$, although the Fermi surface is modified by the antiferromagnetic Brillouin zone boundaries. In $CeIn_3$, the detected dHvA branch named d is very close to that of $LaIn_3$. On the other hand, a large sherical Fermi surface centered at the R point, which is observed in $LaIn_3$, is not observed in $CeIn_3$. This is due to the folding of the magneitc Brillouin zone.

In the present study, we reports the change of the Fermi surface in $CeIn_3$ undre pressure up to 3 GPa. The large spherical Fermi surface named a appears in the pressure region $P > P_c \simeq 2.6\,GPa$. Comparing the dHvA frequency of this Fermi surface to the experimental values of $LaIn_3$ and $ThIn_3$ and also the theoretical values of band energy calculations for $LaIn_3$ and a $4f$-itinerant $CeIn_3$, it is concluded that the $4f$ character in $CeIn_3$ changes from localized to itinerant at P_c, as observed in $CeRh_2Si_2$ and $CeRhIn_5$. In other word, the Fermi surface changes from the small Fermi surface to the large Fermi surface at the P_c in these compounds. Namely, one electron is added to the volume of the Fermi surface for $CeIn_3$ above P_c. We also note that the cyclotron mass m_c^* of this main Fermi surface in $CeIn_3$ is extremely enhanced around P_c: $m_c^* \simeq 60m_0$ at 2.7 GPa for $H \parallel \langle 100 \rangle$, which is compared to $m_c^* = 0.59m_0$ in $ThIn_3$. The field dependence of the cyclotron mass will be also discussed.

[1] N. D. Mathur, F. M. Grosche, S. R. Julian, I. R. Walker, D. M. Freye, R. K. W. Haselwimmer and G. G. Lonzarich: Nature **394** , (1998) 39.

PA33

A drastic change of the Fermi surface in $CeRhIn_5$ and $CeRh_xIr_{1-x}In_5$

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We carried out the de Haas-van Alphen experiments for $CeTIn_5$ (T : Co, Rh and Ir) and $CeRh_xIr_{1-x}In_5$ both ambient and under pressure. $CeTIn_5$ has the unique tetragonal crystal structure with alternating layers of $CeIn_3$ and TIn_2, stacked sequentially along the [001] direction. Reflecting this crystal structure, $CeTIn_5$ has the quasi-two dimensional electronic states, namely the corrugated cylindrical Fermi surfaces. Fermi surfaces of $CeRhIn_5$ are approximately the same as those in a non-$4f$ $LaRhIn_5$ at ambient pressure. On the other hand, the Fermi surfaces of $CeCoIn_5$ are well explained by the $4f$ itinerant energy band calculation. A drastic change of the Fermi surfaces in $CeRhIn_5$ occurs when the pressure crosses $P_c \simeq 2.35\,\mathrm{GPa}$ [1]. Fermi surfaces of $CeRhIn_5$ change from $LaRhIn_5$-like Fermi surfaces ($P < P_c$) to $CeCoIn_5$-like Fermi surfaces ($P > P_c$), as shown in Fig. 1. We also observed a similar change of the Fermi surfaces in $CeRh_xIr_{1-x}In_5$ at about $x = 0.3$.

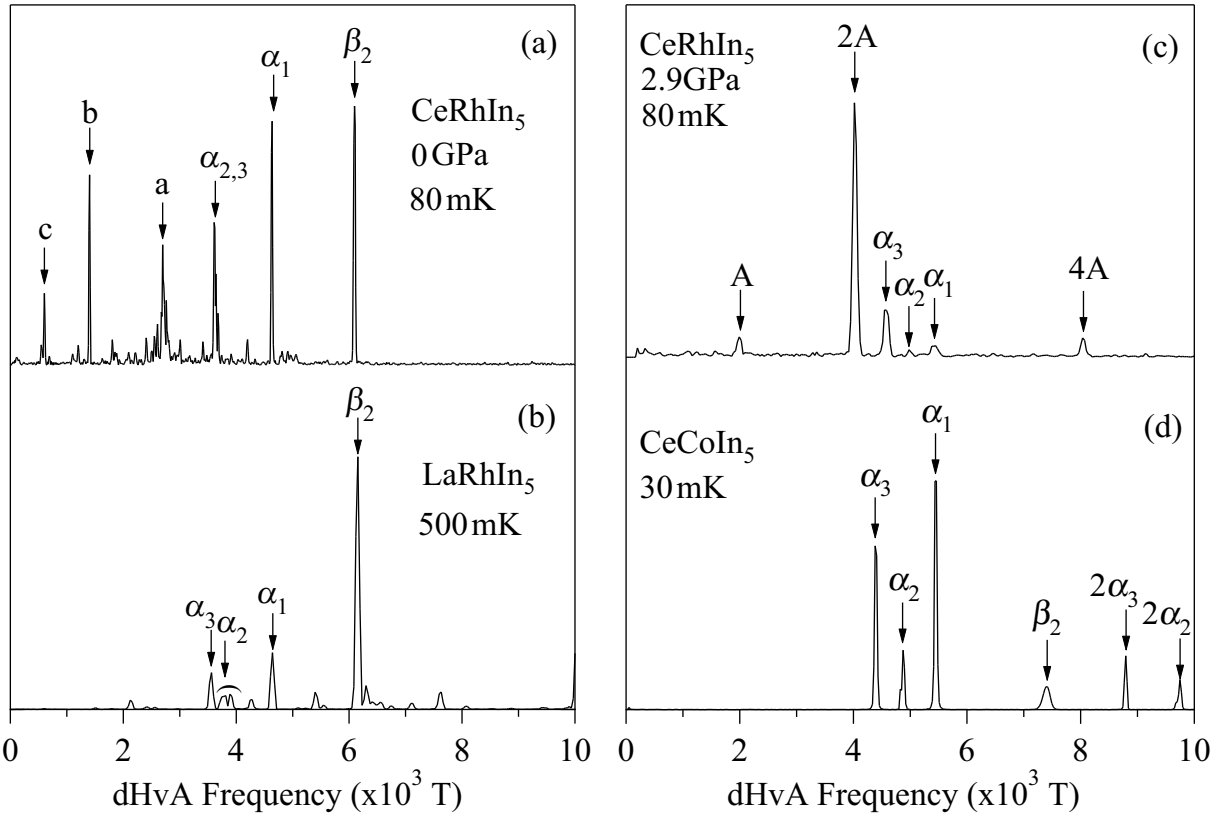

Figure 1: FFT spectra in (a) $CeRhIn_5$ at 0 GPa, (b) a non-$4f$ $LaRhIn_5$, (c) $CeRhIn_5$ at 2.9 GPa and (d) $CeCoIn_5$ at 0 GPa.

[1] H. Shishido, R. Settai, H. Harima and Y. Ōnuki, J. Phy. Soc. Jpn. **74**, (2005) 1103.

PA34

^{115}In-NQR study of heavy fermion compound Ce_2RhIn_8

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Ce_2RhIn_8 is a heavy fermion compound: at ambient pressure, it is an antiferromagnet with T_N = 2.8 K [1]. It becomes superconducting below 1.4 K at 2.0 GPa. Its crystal structure can be viewed as the successive layers of the heavy fermion compounds $CeRhIn_5$ (T_{SC} = 2.2 K at 2.5 GPa) [2] and $CeIn_3$ (T_{SC} = 0.25 K at 2.5 GPa) [3]. Since the T_{SC} of Ce_2RhIn_8 exists between those of the corresponding $CeRhIn_5$ and $CeIn_3$, it is quite important to study its electronic state in consideration for the dimensionality of the system [4,5]. In order to reveal its physical properties more microscopically, we have performed nuclear quadrupole resonance (NQR) measurement on ^{115}In nuclei of Ce_2RhIn_8. Spin-lattice relaxation rate $1/T_1$ of Ce_2RhIn_8 under pressure of about 2 GPa decreases with decreasing temperature T and is proportional to $T^{1/2}$ just above T_{SC}. This is contrast with the T-linear dependence of the $1/T_1$ of Ce_2CoIn_8 at low temperatures [6]. In our poster, we will also discuss the T dependence of $1/T_1$ at lower temperatures.

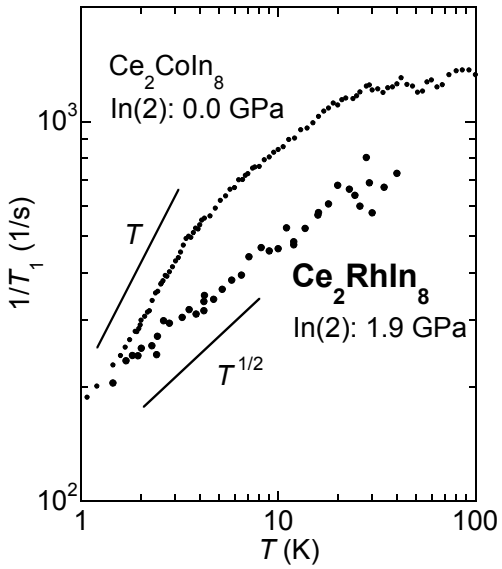

Figure 1: Spin-lattice relaxation rate of Ce_2TIn_8 (T=Co, Rh).

[1] M. Nicklas *et al.*: Phys. Rev. B **67** (2003) 020506(R).
[2] H. Hegger *et al.*: Phys. Rev. Lett. **84** (2000) 4986.
[3] N. D. Mathur *et al.*: Nature **394** (1998) 39.
[4] T. Takimoto and T. Moriya: Phys. Rev. B **66** (2002) 134516.
[5] H. Fukazawa and K. Yamada: J. Phys. Soc. Jpn. **72** (2003) 2449.
[6] H. Fukazawa *et al.*: Physica B **359-361** (2005) 181.

PA35

Thermodynamic Study on the Heavy Fermion Superconductor under High Pressure.

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M. Nakashima[2] A. Thamizhavel[2], T. Takeuchi[2], R. Settai[2] and Y. Onuki[1,2]

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In this workshop, we will show our recent investigations on the heavy femion superconductors by the ac calorimetry method under pressure. The method is powerful tool since the high sensitive measurement of the heat capacity is possible.

Bauer *et al.* reported superconductivity in $CePt_3Si$ with the non-centrosymmetric tetragonal structure (space group $P4\ mm$)[1]. Superconductivity with the transition temperature $T_{sc} = 0.75$ K is realized in the long-range antiferromagnetic ordered state with the Néel temperature $T_N = 2.2$ K. We determine the pressure phase diagram of $CePt_3Si$ as shown in the figure 1[2]. The Néel temperature decreases with increasing pressure and becomes zero at the critical pressure $P_{AF} \simeq 0.6$ GPa. On the other hand, the superconducting phase exists in a wider pressure region from ambient pressure to about 1.5 GPa. The superconducting phase consists of two regions from 0 to $P_{AF} \simeq 0.6$ GPa and from P_{AF} to 1.5 GPa. There is no anomalous singular behavior in the pressure dependences of the electronic specific heat coefficient γ or the coefficient of the T^2 term in the resistivity A around P_{AF}. This suggests that the superconductivity in $CePt_3Si$ differs from those observed around the quantum critical point such as in $CeIn_3$.

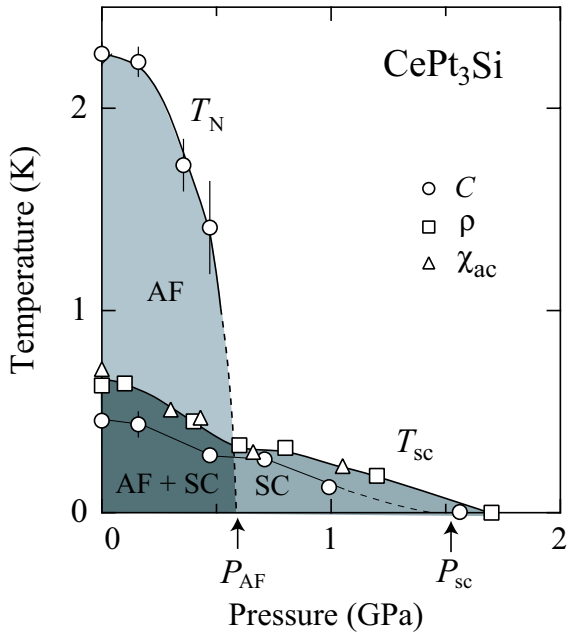

Figure 1: Pressure phase diagram in $CePt_3Si$

[1] E. Bauer *el al.*, Phys. Rev. Lett.: **92**, (2004) 027003.
[2] N. Tateiwa *el al.*, J. Phys. Soc. Jpn.: **74**, (2005) 1903.

PA36

Pressure effect on magnetism and superconductivity in $CePt_3Si$

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Magnetism and superconductivity in the heavy fermion superconductor $CePt_3Si$[1] have been studied under pressure. The antiferromagnetic transition temperature T_N decreases by applying pressure and becomes zero at 0.6 - 0.7 GPa[2]. On the other hand, the superconducting transition temperature T_{sc} decreases with increasing pressure and becomes zero in the pressure range 1.2 - 1.7 GPa, as shown in Fig. 1. Interestingly, the pressure dependence of T_{sc} in Fig. 2 exhibits a shoulder-like feature around 0.7 GPa. Another characteristic temperature T_{max} $\sim$5 K at ambient pressure, which was observed in the magnetic specific heat and thermal expansion coefficient[2], was found to shift to higher temperatures above 0.7 GPa. These results are summarized in Fig. 2 and suggest that a critical pressure exists around 0.7 GPa in $CePt_3Si$.

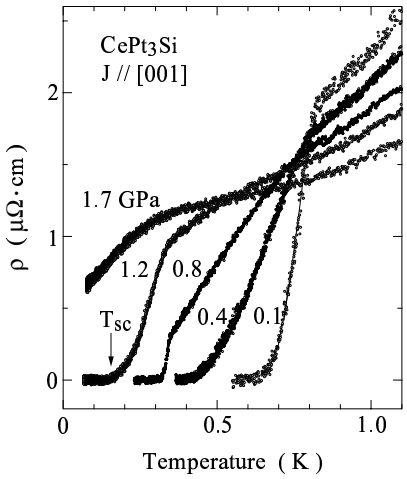

Figure 1: Temperature dependence of the electrical resistivity under several pressures in $CePt_3Si$. T_{sc} is defined as the temperature at which the resistivity becomes zero.

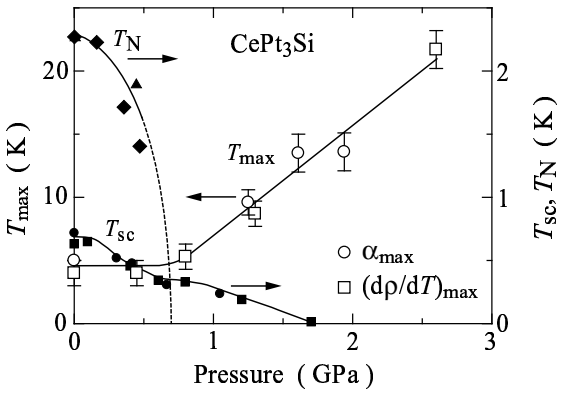

Figure 2: Temperature dependence of T_{max}, T_N and T_{sc} in $CePt_3Si$.

[1] E. Bauer *et al*, Phys. Rev. Lett. **92** (2004) 027003-1.
[2] N. Tateiwa *et al*, J. Phys. Soc. Jpn. **74** (2005) 1903.
[3] T. Takeuchi *et al*, J. Phys.: Condens. Matter **16** (2004) L333.

PA37

Superconductivity in the antiferromagnetic state of $CeNiGe_3$

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[2] *Dept. Elect. & Elect. Eng., Muroran Institute of Technology , Mizumoto, Muroran 050-8585, Japan*
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$CeNiGe_3$ orders antiferromagnetically at $T_N = 5.5$ K with localized $4f$ magnetic moments at ambient pressure. We have performed the resistivity measurement for the polycrystal sample under high pressure up to 10 GPa using Daphne oil (7373) as the pressure-transmitting medium.

The T_N initially increases with increasing pressure up to 3 GPa, suggesting that the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction is dominant rather than the Kondo effect below ~ 3 GPa. The T_N becomes zero at a quantum critical point (QCP) that is located at approximately $6-7$ GPa. We found that superconductivity occurs in the antiferromagnetic (AF) phase well removed from the QCP, in addition to around the QCP. [1] The coefficient of A in $\rho(T) = \rho_0 + AT^2$ has the maximum value at the QCP, and it has relatively large value even in the AF phase around 3 GPa. Superconductivity is realized even below 3 GPa with the f-localized scheme, in contrast to other Ce-based heavy fermion superconductors. This superconductivity in the AF state rebuts the common idea that spin fluctuations around the QCP are a driving force for the superconductivity.

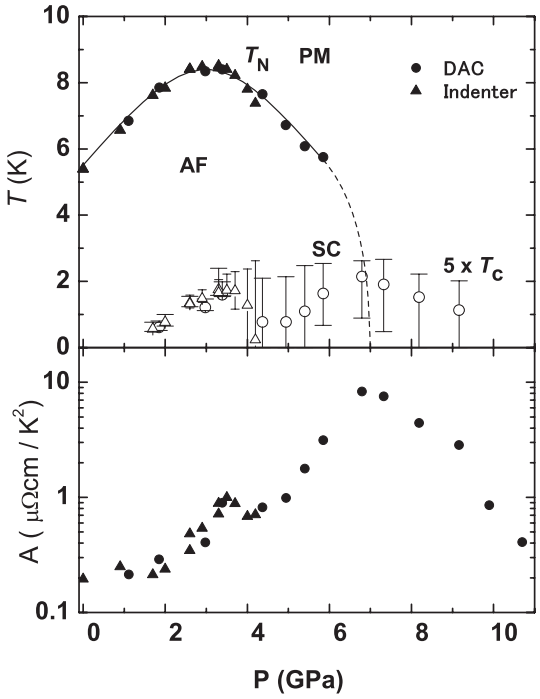

Figure 1: Pressure dependence of T_N, T_c and A.

[1] M. Nakashima et al., J. Phys.: Condens. Matter 16（2004）L255-L262.

PA38

Pressure effect of electrical resistivity in CePtAl

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CePtAl crystallizes in the orthorhombic TiNiSi-type structure. There are three successive magnetic transitions at T_1 = 5.9 K, T_2 = 4.3 K, T_3 = 2.2 K [1,2,3]. At 1.5 K, the canted ferromagnetism with an ordered moment of 1.35 μ_B/Ce oriented parallel to the a-axis is clarified by neutron diffraction, studied from the viewpoint of frustrated magnetism.

Pressure experiment has been done by using the cubic anvil up to 8 GPa down to 2 K [4]. T_1 increases by increasing pressure and disappears at 6.0 GPa, as shown in Fig 1. The A- and ρ_0- values in the T^2-dependence of electrical resistivity have maximum around 6.0 GPa. These results indecate that the electronic state is changed around the critical pressure region. Much lower temperature experiment has required for deeper understanding. Furthermore we have measured the electrical resistivity down to 60 mK up to about 9.0 GPa by using the diamond anvil cell. We will present the experimental result at lower temperatures in the workshop.

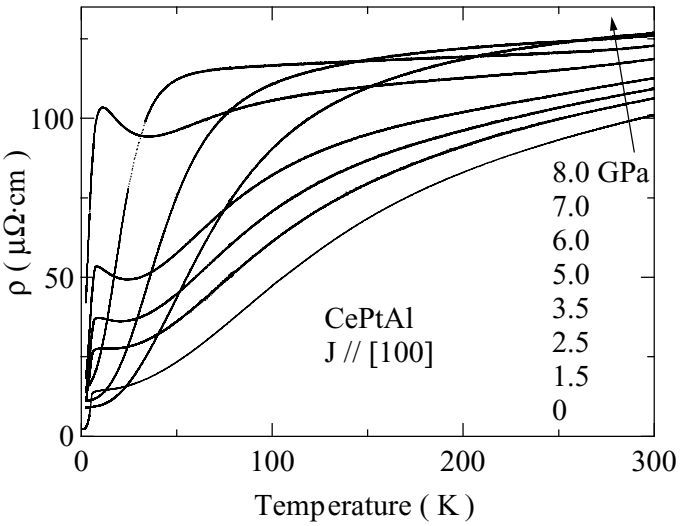

Figure 1: Temperature dependence of electrical resistivity under pressure in CePtAl.

[1] A. Dönni *et al*, J. Phys. Cond. Matt. **7**, (1995) 1663.
[2] H. Kitazawa *et al*, Physica B **237**, (1997) 5678.
[3] H. Kitazawa *et al*, J. Solid State Chem. **140**, (1998) 233.
[4] T. Ueda *et al*, printed in J. Phys. Soc. Jpn.

PA39

Symmetry Breaking Superconductivity in UIr

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[2] *Faculty of Maritime Sciences,Kobe University, Hyogo 658-0022, Japan*
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[4] *Graduate School of Science Osaka University, Osaka 560-0043, Japan*

A ferromagnet UIr, which shows superconductivity under high pressure (P),[1] has the crystal structure without the inversion symmetry. Measuring ac susceptibility, we found three kinds of FM phases (FM1, FM2 and FM3) under high pressure (Fig. 1(a)). In the resistivity measurements, the phase transition of the FM1 and the FM3 can be detected as a kink, but that of the FM2 does not follow any anomaly. In addition, UIr exhibits an anisotropic electrical conductivity at low temperature (T) in the P range of the FM2 phase. Figure 1(b) shows the P dependence of the residual resistivity for J//[10$\bar{1}$] and J//[010]. For J//[010], the residual resistivity at the FM2 becomes ten times larger than that at the FM1, while it doesn't almost change for J//[10$\bar{1}$]. These suggest that the FM2 phase obviously differs from other FM phases.

We observed the FM3 transition and the superconductivity at the same P in the ac-susceptibility measurement. The superconductivity and the FM3 disappear simultaneously with increasing P. These experimental facts suggest that the superconducting phase is included in the FM3 phase. This superconductivity is considered to be realized without both the inversion symmetry and the time reversal symmetry. It is interesting issue how the Cooper pairs are formed in such situation.

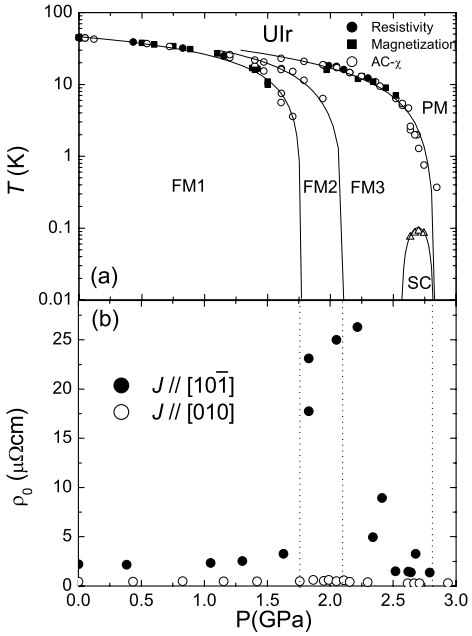

Figure 1: (a) $P-T$ phase diagram (b) the P dependence of the residual resistivity.

[1] T. Akazawa et al., J. Phy. Soc. Jpn., **73**, (2004) 3129.

PA40

Pressure-induced superconductivity in noncentrosymmetric heavy-fermion antiferromagnet $CeRhSi_3$

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[2] *National Institute for Materials Science, Tsukuba, Ibaraki 305-0047, Japan*

We present the pressure-induced superconductivity in a non-centrosymmetric heavy-fermion antiferromagnet $CeRhSi_3$. $CeRhSi_3$ crystalizes in $BaNiSn_3$-type structure belonging to the space group $I4mm$ (No. 107) without inversion center (Fig. 1(a)) With increasing pressure, the Néel temperature (T_N=1.6 K at ambient pressure) initially increases, subsequently decreases above about 7 kbar and becomes unclear above 20 kbar. The superconductivity emerges above about 12 kbar even though the antiferromagnetic ordering persists (Fig. 1(b)). Furthermore, another anomaly is observed in the superconducting phase. The anomalous magnetic field-temperature phase diagram with a high upper critical field suggests that an unconventional superconductivity is realized in $CeRhSi_3$.

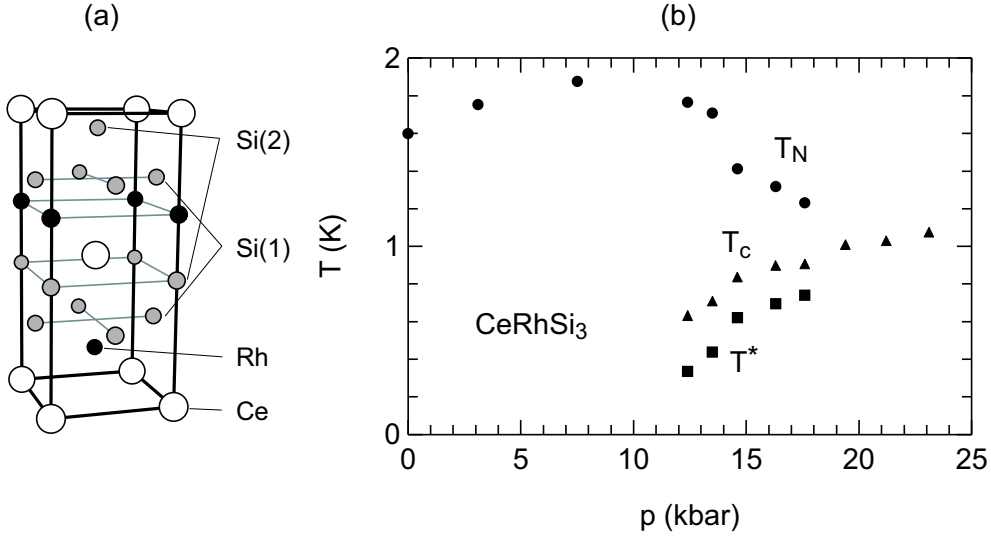

Figure 1: (a)Crystal structure and (b)temperature-pressure phase diagram of $CeRhSi_3$.