Structural Properties of Ce-115 Heavy Fermion Compounds under Pressure

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Introduction

The discovery of a new family of Ce-based heavy fermion superconductors [1-3] that exhibits interesting magnetic and transport properties has triggered much attention toward research on strongly correlated electron compounds. $CeRhIn_5$ changes from an antiferromagnetic ground state to a superconducting state upon the application of a critical pressure P_c of 1.6 GPa. Isostructural $CeCoIn_5$ and $CeIrIn_5$ belong to the same family and are found to be ambient-pressure superconductors. The power-law temperature dependence observed in the specific-heat and thermal-conductivity measurements below the critical temperature T_c strongly suggests the unconventional nature of superconducting behavior and the origin of the non-Fermi liquid state in this class of systems.

The unusual properties reported in these compounds are strongly related to the interactions between the magnetic moments of the f electrons with the conduction electrons. In addition, the closeness of the system to the magnetic instability region called the quantum critical point (QCP) and the reduced dimensionality favor superconductivity. Pressure and doping are regarded as important parameters that are used as the driving forces for suppressing the antiferromagnetic ordering and also for tuning the interactions between the electrons by changing the electronic configuration. In order to understand the influence of pressure on structural parameters, we have performed high-pressure x-ray diffraction on these compounds.

Methods and Materials

X-ray diffraction experiments were conducted at different pressures by using a Merrill-Bassett-type diamond anvil cell at beamline station 16-ID-B at the APS. Single crystals grown by flux technique were finely ground and loaded into a stainless-steel or rhenium gasket with a hole having a diameter of 185 μm. Silicone oil (polydimethylsiloxane) was used as a pressure-transmitting medium, and ruby/NaCl was used for pressure calibration.

The images obtained were integrated by using the software FIT2D, and the refinements were carried out by using the Rietveld program RIETICA [4].

Results

The c/a ratio and normalized volume with respect to pressure for the systems are shown in Fig. 1. The bulk modulus (B_0) and the pressure derivative (B_0') were determined by fitting the pressure and volume (P-V) data by using the Murnaghan equation of state. The bulk modulus values were found to be 72.4, 78.4, and 84 GPa for $CeCoIn_5$, $CeRhIn_5$, and $CeIrIn_5$, respectively.

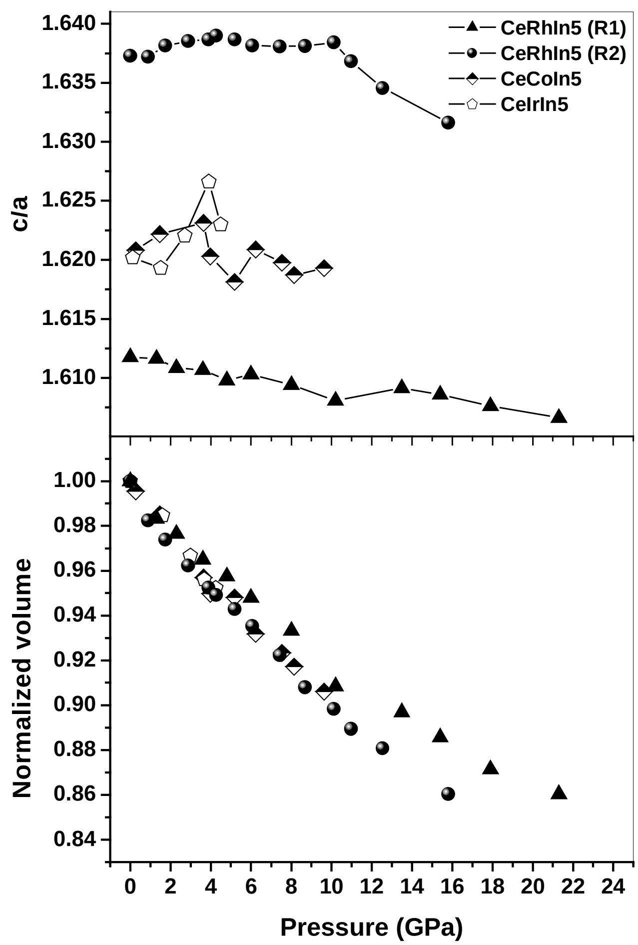

FIG. 1. P-V data and c/a ratio for the Ce 115 compounds. R1 and R2 (in parentheses) indicate different pressure runs.

Discussion

The structural data at high pressures for the Ce-115 are compared with the transport measurements reported earlier [4, 5]. The c/a ratio, which is considered to be an important parameter in discussing the transition temperatures in most of the high-T_c and heavy fermion superconducting systems, is found to exhibit a double-peaked structure with a local minimum around 4 to 5 GPa for $CeRhIn_5$. In accordance with the results from resistivity studies under pressure where an increase in Tc with an increase in the c/a ratio is reported, the structural investigations indicate an indirect relationship with c/a and the transition temperature. Even though the rise in c/a is not strongly pronounced in the case of $CeCoIn_5$, a broad maximum that starts around 1.5 GPa was found and may be related to the hybridization effects. The bulk modulus values calculated for Ce-115 agree well with the reported values for other heavy fermion compounds [6].

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References

[1] H. Hegger, C. Petrovic, E.G. Moshopoulou, M.F. Hundley, J.L. Sarrao, Z. Fisk, and J.D. Thompson, Phys. Rev. Lett. **84**, 4986 (2000).

[2] C. Petrovic, P.G. Pagliuso, M.F. Hundley, R. Movshovich, J.L. Sarrao, J.D. Thompson, Z. Fisk, and P. Monthoux, J. Phys.: Condens. Matter **13**, L337 (2001).

[3] C. Petrovic, R. Movshovich, M. Jaime, P.G. Pagliuso, M.F. Hundley, J.L. Sarrao, Z. Fisk, and J.D. Thompson, Europhys. Lett. **53**, 354 (2001).

[4] C.J. Howard and B.A. Hunter, *RIETICA, A Computer Program for Rietveld Analysis of X-ray and Neutron Powder Diffraction Patterns* (Lucas Height Research Laboratories, Lucas Heights, Australia, 1998), pp. 1-27.

[5] T. Muramatsu, N. Tateiwa, T.C. Kobayashi, A. Shimizu, K. Amaya, D. Aoki, H. Shishido, Y. Haga, and Y. Onuki, J. Phys. Soc. Jpn. **70**, 3362 (2001).

[6] V.A. Siderov, M. Nicklas, P.G. Paluso, J.L. Sarrao, Y. Bang, A.V. Balatsky, and J.D. Thompson, Phys. Rev. Lett. **89**, 157004 (2002).

[7] M.F. Hundley, J.L. Sarrao, Z. Fisk, J.D. Thompson, I.L. Spain, F. Steglich, U. Rauchschwalbe, and H.D. Hochheimer, Physica B **139-140**, 449 (1986).