

Low-temperature, High-pressure X-ray Diffraction Studies on CeRhIn₅

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Introduction

Superconductivity observed after the ground-state properties of Ce-based heavy fermion compounds are altered upon the application of pressure has generated wide interest on the relationship between the structure and superconducting properties of this class of compounds [1]. CeRhIn₅ is antiferromagnetic at ambient conditions and becomes superconducting at a pressure of 1.6 GPa with a critical temperature T_c of 1.6K [2]. The superconducting state appears at the point where long-range magnetic ordering is suppressed by pressure as a result of the competing RKKY interactions and the Kondo effect.

CeRhIn₅ crystallizes in the HoCoGa₅ structure with the alternating layers of Ce-In and Rh-In stacked along the c axis. The doping experiments on CeMIn₅ (M = rare earth) and the uniaxial pressure experiments at low temperatures show a direct relationship between the structural parameters and the superconducting properties [3, 4]. CeRhIn₅ is an ideal candidate for pressure investigations because the transport and structural data have been studied in detail and also because it exhibits pressure-induced superconductivity. To investigate the effect of pressure on the structure close to the superconducting regime, we planned to perform a low-temperature x-ray diffraction (XRD) experiment at high pressures.

Methods and Materials

CeRhIn₅ single crystals were grown by a self-flux technique. The single crystals were crushed into powder. XRD measurements showed the single-phase nature of the compound. In agreement with previous results, the crystals were found to have tetragonal symmetry with cell parameters $a = 4.6531 \pm 0.0001$ Å and $c = 7.5538 \pm 0.0009$ Å. A Merrill-Bassett-type diamond anvil cell with a stainless-steel gasket having a hole with a diameter of 185 μ m and an indentation thickness of 60 μ m was used for the experiment. The finely ground powder was pressed into a pellet, and a small piece was cut from it and loaded in the gasket hole with an Au pressure marker and silicone oil. The diamond anvil cell was then placed inside a continuous-flow-type cryostat with a pressurizing device. The cryostat was precooled with liquid nitrogen at temperatures around 10K and stabilized by pumping liquid He. The temperature was maintained at 10K throughout the experiment.

XRD patterns were collected at different pressures up to 8 GPa at beamline station 16-ID-B at the APS. The x-ray patterns obtained were integrated by using FIT2D, and the structural refinement was done with the Rietveld program RIETICA.

Results

The diffraction patterns collected at different pressures at 10K are shown in Fig. 1. The pressure and volume (P-V) data and the variations of c/a with pressure for CeRhIn₅ are shown in Fig. 2. The c/a ratio is found to have a double maximum structure, similar to that found in the room-temperature, high-pressure XRD measurements. The bulk modulus value $B_0 = 78.2 \pm 5.2$ GPa obtained by fitting the P-V data to the Murnaghan equation is identical to the room-temperature value within the experimental uncertainty.

In previous reports, a strong correlation between the ambient pressure c/a ratio and the critical temperature T_c in the CeMIn₅ compounds was observed (increasing c/a increases T_c) [3]. In the low-temperature experiment, the c/a plot with respect to pressure shows a significant enhancement of c/a around 6.9 GPa. Even though there is no direct correlation linking the T_c with c/a in our

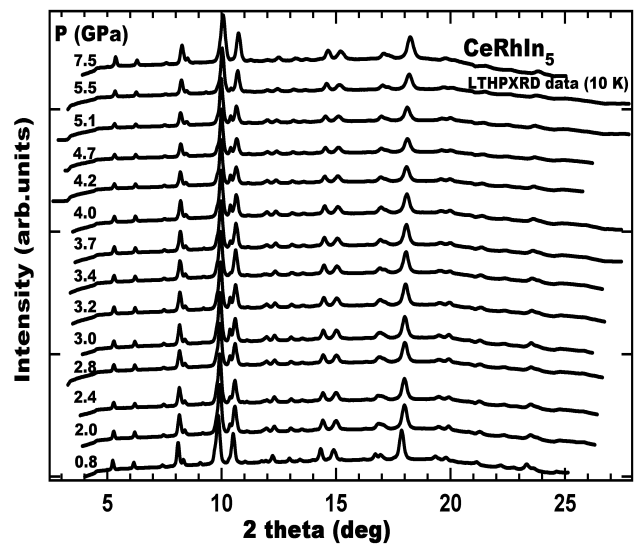


FIG. 1. X-ray diffraction patterns at different pressures for CeRhIn₅ at 10K.

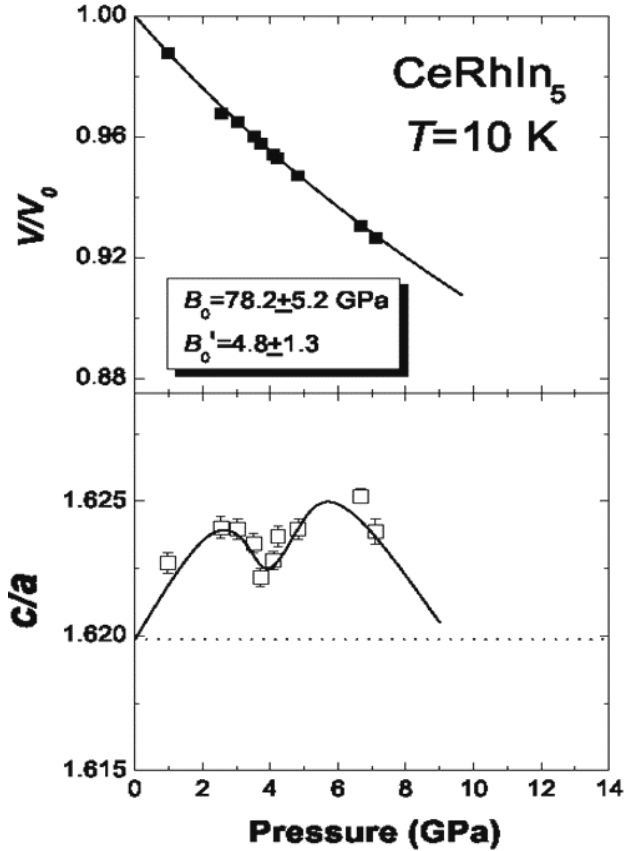


FIG. 2. P - V data and c/a ratio with respect to pressure for CeRhIn_5 .

experiments, the value of c/a (1.624) where $T_c(P)$ has its maximum at a pressure of around 2.5 GPa is consistent with a correlation between the room-temperature value of c/a and T_c for various CeMIn_5 compounds [5]. This leads to the natural conclusion that hybridization effects are

likely the driving force behind the observed $T_c(P)$ behavior in CeRhIn_5 .

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References

- [1] N.D. Mathur, F.M. Grosche, S.R. Julian, I.R. Walker, D.M. Freye, R.K. Haselwimmer, and G.G. Lonzarich, *Nature* **394**, 39 (1998).
- [2] 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).
- [3] P.G. Pagliuso, R. Movshovich, A.D. Bianchi, M. Nicklas, N.O. Moreno, J.D. Thompson, M.F. Hundley, J.L. Sarrao, and Z. Fisk, *Physica B* **312-313** 129 (2002).
- [4] N. Oeschler, P. Gegenwart, M. Lang, R. Movshovich, J.L. Sarrao, J.D. Thompson, and F. Steglich, *Phys. Rev. Lett.* **91**, 076402 (2003).
- [5] R.S. Kumar, H. Kohlmann, B.E. Light, A.L. Cornelius, V. Raghavan, T.W. Darling, and J.L. Sarrao, *Phys. Rev. B*, <http://arxiv.org/pdf/cond-mat/0209005> (accepted for publication, 2003).