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Structural Phase Transition in $CePd_2Ga_2$ under Hydrostatic Pressure

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The structural phase transition from tetragonal to triclinic structure in $CePd_2Ga_2$ compound was studied by means of electrical resistivity measurement under hydrostatic pressure. The shift of the transition to the higher temperature with increasing pressure was revealed: 195 K in 3 GPa compared to 125 K in ambient pressure.

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1. Introduction

CeT_2X_2 family of compounds (T = d-element and X = p-element) has been intensively studied for many years because of such physical properties as a superconductivity, pressure-induced superconductivity or non-Fermi liquid behaviour at low temperatures. Another interesting feature was observed in $CePd_2Al_2$: the presence of an additional peak in inelastic neutron spectra [1]. This peak originates in a strong electron–phonon coupling forming a new quasi-bound state, so called vibron state [2].

CeT_2X_2 compounds crystallize mostly in tetragonal structures of $ThCr_2Si_2$-type and $CaBe_2Ge_2$-type. The compounds crystallizing in the latter structure type are often structurally unstable and exhibit the phase transition to structure with lower symmetry [1, 3, 4]. The c/a ratio could be introduced as an important criterion for the stability of crystal structure. The value of c/a smaller than 2.3 indicates a structural instability in the compound [3]. $CeCu_2Sn_2$ (c/a = 2.34) [5] and $CeIr_2Ge_2$ (c/a = 2.38) [6] reveal stable tetragonal structure, whereas $CePt_2Ge_2$ (c/a = 2.23) [7], $CeNi_2Sn_2$ (c/a = 2.29) [5], $CePd_2Ga_2$ (c/a = 2.22) [3] and $CePd_2Al_2$ (c/a = 2.24) [3] undergo a structural phase transition.

The presented work is focused on $CePd_2Ga_2$ compound crystallizing in tetragonal $CaBe_2Ge_2$-type structure. With the value of c/a ratio around 2.22 [3], $CePd_2Ga_2$ belongs to the group of structurally unstable compounds. The structural phase transition from tetragonal to triclinic structure was observed at 125 K [3, 8]. Somewhat lower transition temperature was observed also in the La counterpart (62 K) [3,8], revealing the same type of structural transition. The influence of the Al–Ga substitution on structural and electronic properties of $CePd_2Ga_2$ was investigated in our recent study [8]. The transition temperature is shifted to lower temperature with increasing Al content, while the c/a ratio increases. Our study deals with the electronic properties of $CePd_2Ga_2$ compound studied by means of electrical resistivity under hydrostatic pressure. Hydrostatic pressure represents another way to change physical properties, moreover, without the change of electronic structure.

2. Experimental methods

The $CePd_2Ga_2$ compound was prepared by arc-melting of pure elements (Ce — 2N8, Pd — 3N5, Ga — 7N) in a mono-arc furnace under protective argon atmosphere. The sample was turned and remelted four times to obtain better homogeneity. Prepared sample was additionally sealed in quartz tubes and annealed for 10 days at 850 °C.

The crystal structure and sample quality were investigated by powder X-ray diffraction and electron microscopy at room temperature. The analysis of diffraction patterns was done using FullProf program employing the Rietveld method [9]. The $CaBe_2Ge_2$-type structure (space group 129) was confirmed with the following lattice parameters: a = 4.425(4) Å, c = 9.845(7) Å, c/a = 2.224(6), well in agreement with previous results [3]. The energy dispersive X-ray diffraction verified expected chemical composition and stoichiometry.

The He Closed Cycle cryostat (Janis Research) and classical AC four-probe method were used for the measurement of the electrical resistivity under hydrostatic pressure. The double layered cylindrical pressure cell and pressure exchange medium Daphne 7373 oil [10] were used for the measurement up to 3 GPa in temperature range 4–300 K. The manganin wire was used as the pressure sensor. The pressure was determined at room temperature with an error of 0.05 GPa and with higher uncertainty (≈ 0.2 GPa) above 2.2 GPa and below 1 GPa because of the solidification of Daphne 7373 oil [10].

3. Results and discussion

The temperature dependence of electrical resistivity of $CePd_2Ga_2$ under hydrostatic pressure is shown

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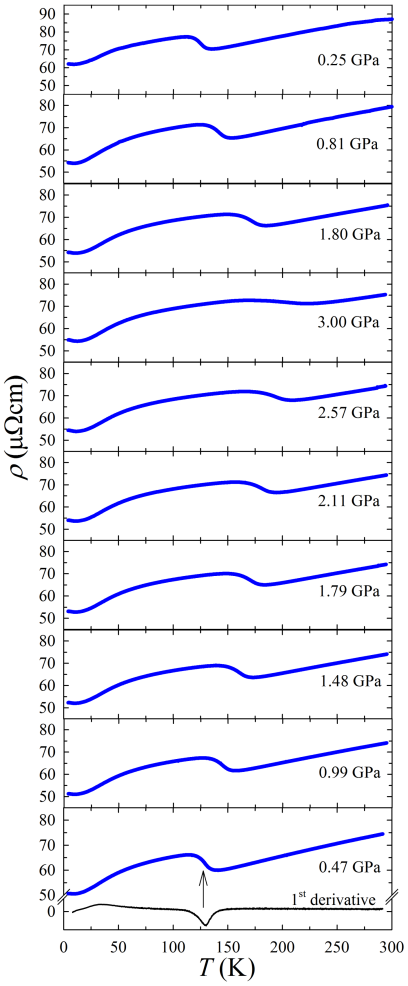

Fig. 1. The electrical resistivity measured on $CePd_2Ga_2$ under hydrostatic pressure. The data for pressure points are given in order they were measured (0.47 → 3.00 → 0.25 GPa). The arrow marks the minimum point of the derivative determining the transition temperature.

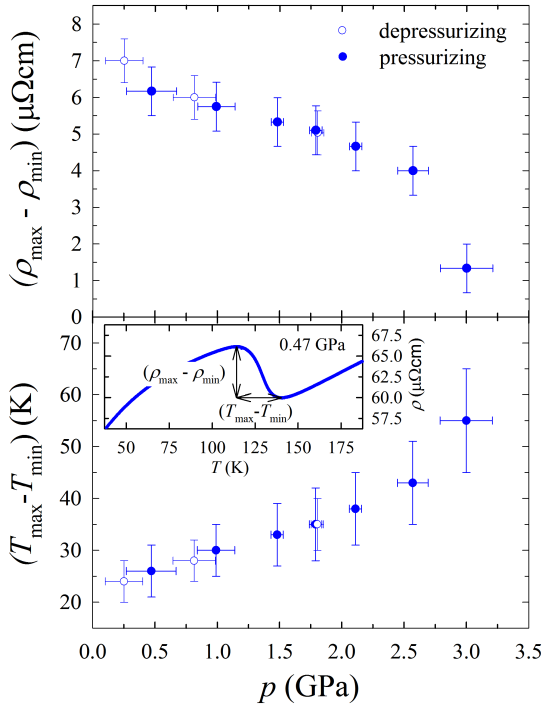

Fig. 2. Parameters $(\rho_{\max} - \rho_{\min})$ and $(T_{\max} - T_{\min})$ of the anomaly (connected with structural transition) observed in resistivity data for CePd2Ga2. The insert contains an illustration of these parameters.

in Fig. 1. The electrical resistivity was measured in cooling and heating regimes without any significant difference between those two regimes (the data for heating regime are not shown). The measurements were performed in order presented in Fig. 1, i.e. in pressures from 0.47 to 3.00 GPa and back from 3.00 to 0.25 GPa. The shape of anomaly on electrical resistivity curve connected with the structural phase transition (around 127 K for 0.47 GPa) is well in agreement with previously published results [3, 8]. The parameters of the anomaly bounded with structural transition are presented in Fig. 2 for illustration. The local minimum–maximum distance in temperature and in resistivity, $T_{\max} - T_{\min}$ and $\rho_{\max} - \rho_{\min}$, respectively, are shown in Fig. 2. The anomaly becomes broader in temperature and related resistivity change becomes smaller with increasing pressure. The temperature of structural phase transition is determined from minimum of the first derivative, see measurement in 0.47 GPa in Fig. 1 as an example.

The obtained phase diagram is presented in Fig. 3. The temperature of structural phase transition, T_{str}, develops almost linearly with increasing hydrostatic pressure in the whole pressure region (0.48–3.00 GPa). The data are fitted to the linear function $T = ap + b$ resulting in values of $a = (28 \pm 1)$ K(GPa)$^{-1}$ and $b = (120 \pm 2)$ K to quantify observed $T(p)$ dependence. The temperature of structural phase transition obtained by electrical resistivity measurement without pressure cell (taken from Ref. [8]) is shown in Fig. 3 as well. This value fits relatively well to the observed $T(p)$ dependence.

Let us compare the influence of hydrostatic pressure and chemical pressure [8] on $CePd_2Ga_2$ compound. The structural phase transition is shifted to lower temperatures with increasing Al content in the $CePd_2Al_{2-x}Ga_x$ [8], whereas the increase of transition temperature is observed with the application of hydrostatic pressure on $CePd_2Ga_2$. Such behaviour can be tentatively related to the development of the c/a ratio. The c/a is decreasing with increasing Ga content in $CePd_2Al_{2-x}Ga_x$ series [8]. Continuing this trend our present observation would point to a further decrease of c/a in $CePd_2Ga_2$ with applied hydrostatic pressure. The relation between the temperature of structural transition and c/a ratio seems to be meaningful also with respect to general systematics in this group of materials [3]. The decrease of c/a with applied hydrostatic pressure in

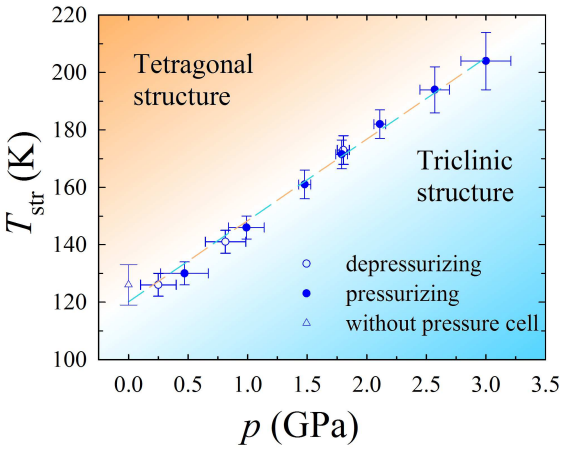

Fig. 3. The phase diagram of CePd2Ga2 with linear fit: $T = ap + b$, where $a = (28 \pm 1)$ K(GPa)$^{-1}$ and $b = (120 \pm 2)$ K. The values were obtained from the data measured in cooling regime (the heating regime reveal identical values). The closed and open circles were determined with pressurising and depressurising, respectively. The open triangle marks the position of T_{str} obtained from measurement without pressure cell taken from Ref. [8].

$CePd_2Ga_2$ would then also imply larger compressibility along the c-axis than along the a-axis in this compound.

4. Conclusions

We investigated the structural phase transition from tetragonal to triclinic structure in $CePd_2Ga_2$ by means of electrical resistivity measurement under hydrostatic pressure. The shift of the transition to the higher temperatures with pressure application is attributed to the change of the lattice parameters, especially then the change of the c/a ratio.

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