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Electrical resistivity under pressure and thermal expansion of LaPt₂Si₂ single crystal

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ABSTRACT

We have performed electrical transport under pressure and thermal expansion measurements on a LaPt₂Si₂ single crystal. The charge density wave (CDW) transition temperature T_{CDW} decreases, while the superconducting transition temperature T_C increases with the application of pressure, which confirms the competing nature of the two phases. We present an attempt to understand the pressure (P) dependence of T_{CDW} within the framework of the mean field theory. A well defined anomaly in temperature-dependent relative thermal expansion ($\Delta L/L_0$) and the linear thermal expansion coefficient (α_a) has been observed around T_{CDW} associated with the structural transformation accompanied by a CDW transition.

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I. INTRODUCTION

The Pt-based rare earth intermetallic series RPt_2Si_2 (R = rare earth element) have close structural resemblance to the pnictide superconductors AFe_2As_2 (A = Ba, Sr, Eu). The layered structure of these materials gives them a quasi-two dimensional Fermi surface (FS), and hence these are likely to have various electronic phases which manifest a charge density wave (CDW),^{1,2} the Kondo effect,^{3,4} unusual magnetic properties,⁵ and superconductivity (SC).⁶ LaPt₂Si₂ (LPS) is one of the members of this series that has CaBe₂Ge₂ type tetragonal structure at room temperature. LPS undergoes a structural transformation from room temperature tetragonal to an orthorhombic structure accompanied by a CDW transition below T_{CDW} along with a superconducting transition at about 1.5 K.² The mechanism of CDW in LPS has been proposed to be q -dependent electron-phonon coupling with quasinesting of the FS by Kim *et al.*⁷ Large hysteresis between heating and cooling data in electrical resistivity, magnetic susceptibility, and specific heat reveals the first order nature of the phase transition associated with CDW.^{8,9} Superlattice reflections associated with the CDW were seen at wave vector, $q = (n/3, 0, 0)$, where $n = 1, 2$ (n is the order of reflection), as revealed by small angle electron diffraction studies.²

A CDW is a periodic spatial modulation of electronic charge density,^{10,11} which couples with ion density to minimize the total energy of a system and results in a gap in the single particle density

of states below the transition temperature. The mechanism for a CDW is predominantly the nesting of the Fermi surface, where occupied states are connected to the unoccupied states by a wave vector $q = 2k_F$, where k_F is the wave vector at the Fermi surface. As a result, the electronic susceptibility given by the Lindhard response function¹² has a maximum at a wave vector q , which can diverge in the 1D limit. This electronic density in the reciprocal space leads to a periodic modulation of the electronic charge density in the real space. Due to electron-phonon coupling in the system, this modulation is shifted to the lattice which brings a new periodicity into account. The new periodicity opens up a gap at the FS.

Thermal expansion (TE) is a powerful technique to probe even a slight change in the lattice parameter associated with various phase transitions. Detailed investigation of anomalies related to CDW has been undertaken in CeOs₂Al₁₀,¹³ R₃Ir₄Si₁₀,¹⁴ NbSe₂,¹⁵ RAgSb₂,¹⁶ etc., through TE studies. We have carried out TE experiments on single crystals of LPS grown using the Czochralski pulling method. A TE experiment was carried out using a high resolution capacitive dilatometer technique with a resolution of approximately 1 Å.

Furthermore, competition between various phases can lead to the emergence of new phenomena, e.g., SC appears in the case of pnictide superconductors at the boundary of antiferromagnetic spin density wave ordering and nonordering states.¹⁷⁻¹⁹ Parent compounds of Fe-pnictides show a spin density wave (SDW) transition

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with no signature of SC, but it appears after the suppression of a SDW through the application of chemical pressure/external pressure and electron/hole doping.^{20–23} The interplay between a CDW and SC has recently been observed in high T_C cuprate superconductors.^{24–26} Transition metal dichalcogenides have been studied well to understand the correlation between the two phases, in particular, TX_2 series, where T stands for the transition metal and X is S, Se, Te.^{27–30} The new systems which show such coexistence are always of great interest. In this context, RPt_2X_2 (R = rare earth elements, Sr, Ba and X = Si, As, Ge) is very intriguing as many of the members of this series undergo a structural transition accompanied by a CDW transition and have a phase diagram similar to the pnictide superconductors. For instance, pressure-dependent transport studies in $BaPt_2As_2$ reveal a rich pressure–temperature phase diagram showing the presence of multiple phase transitions with the application of pressure. LPS can also serve as an ideal system to perform pressure-dependent studies as it shows coexistence of a CDW and SC.^{2,8} The competing nature of the two phases has been revealed by applying chemical pressure through Ge doping in polycrystalline $LaPt_2(Si_{1-x}Ge_x)_2$.⁸ We have performed transport measurement under pressure on a single crystal to get further insights into the interaction between a CDW and SC.

II. METHODS

$LaPt_2Si_2$ melts congruently which makes it possible to grow single crystals using a pulling method. A detailed procedure for the growth of single crystals has been reported earlier.⁹ The crystal structure and the single phase nature of the grown crystal was confirmed through powder X-ray diffraction (XRD) with $Cu - K\alpha$ radiation. Scanning electron microscopy (SEM) along with energy dispersive X-ray spectroscopy (EDX) were used to check the composition and uniformity of the crystal. Laue diffraction was used to orient the crystal along the desired crystallographic directions.⁹ Appropriately shaped specimens were obtained using spark erosion. The change in the length of the sample and coefficient of linear thermal expansion (α) has been measured using a capacitive dilatometric technique as elaborated by K uchler *et al.*³¹ The sample dimension used for thermal expansion experiment was $1.36 \times 1.04 \times 0.82 \text{ mm}^3$. Pressure-dependent electrical resistivity down to 400 mK was measured using a Cu–Be piston cylinder cell. Well established pressure-dependent value of resistivity of manganin was used for determination of the pressure. Daphne 7373 oil was used as a pressure transmitting medium. The dimensions of the sample used for this measurement was $2.42 \times 1.31 \times 0.76 \text{ mm}^3$.

III. RESULTS AND DISCUSSION

A. Transport measurements under pressure

Figure 1 shows the electrical resistivity of the single crystal oriented along the a -axis under pressures ranging from 3.2 to 21.5 kbar. The data were collected during a heating run. $LaPt_2Si_2$ undergoes a CDW transition at around 85 K as evidenced by increase in resistivity before the transition due to opening of a partial gap at the Fermi surface. The anomaly related to charge density wave shifts toward lower temperature, while superconducting transition temperature shifts toward higher temperature with increase of pressure (shown in the P – T phase diagram in the inset of Fig. 1). The above

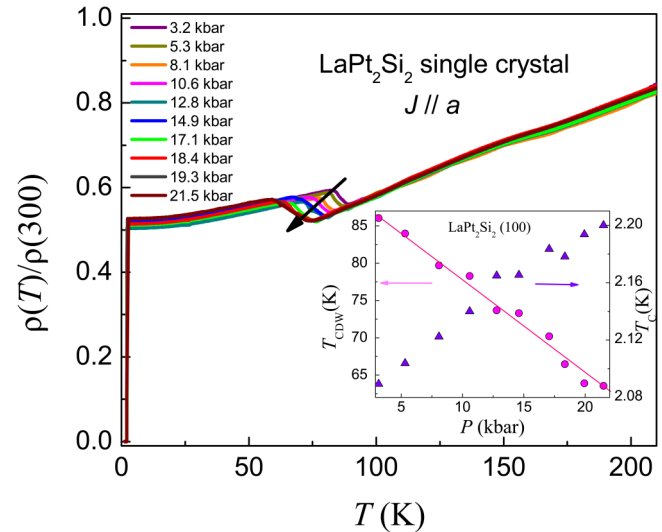


FIG. 1. The temperature dependence of normalized resistivity [$\rho(T)/\rho(300)$] along the a axis of $LaPt_2Si_2$ at different pressures during heating run. The inset shows the P – T phase diagram including pressure dependence of both the transitions. Solid pink line through T_{CDW} vs P curve shows fitting with equation $T_{CDW} = T_0 \exp(-bP)$.

observation confirms the competing nature of the two phases as already claimed in our earlier reports on single as well as polycrystalline $LaPt_2Si_2$.^{8,9} We have drawn a P – T phase diagram based on the above results as shown in the inset of Fig. 1. T_{CDW} has been calculated at the point of minimum in $\frac{d\rho}{dT}$ vs T curve, while T_C is taken as the onset of the superconducting transition. A change of slope was seen around 150 K, which is associated with the solidification temperature of the Daphne 7373 oil,³² used as the transmission medium for hydrostatic pressure.

Within the framework of the mean field theory,³³ the pressure dependence of T_{CDW} is expected to follow an exponential form given by the relation: $T_{CDW} = 5.43 T_F \exp(-1/\lambda)$, where T_F is the Fermi temperature and $\lambda = \omega_q/g^2 N(E_F)$. ω_q represents the phonon frequency, g is the electron–phonon coupling constant, and $N(E_F)$ is the density of states at the Fermi level. With the increase in pressure, due to hardening of phonon spectra, ω_q will increase and as a result a decrease in T_{CDW} is expected. Hence, we fitted T_{CDW} vs P data with an empirical relation, $T_{CDW} = T_0 \exp(-bP)$, which has a form similar to that given by the mean field theory mentioned earlier. The fit parameters are $T_0 = 91(1) \text{ K}$ and $b = 0.0169(8) \text{ kbar}^{-1}$. The value of b is less than what is seen in the CDW compound V_3Te_4 ,³⁴ where $b = 0.025(2) \text{ kbar}^{-1}$. The lower value of b shows the weaker dependence of T_{CDW} on pressure in our system. The rate of change of the two transition temperatures associated with CDW and SC with pressure are $-1.27(5) \text{ K/kbar}$ and $0.0061(3) \text{ K/kbar}$, respectively.

B. Thermal expansion

Figure 2 shows the temperature-dependent relative thermal expansion data ($\Delta L/L_0$, where L_0 is the length of the sample at room temperature) collected for both heating and cooling runs in

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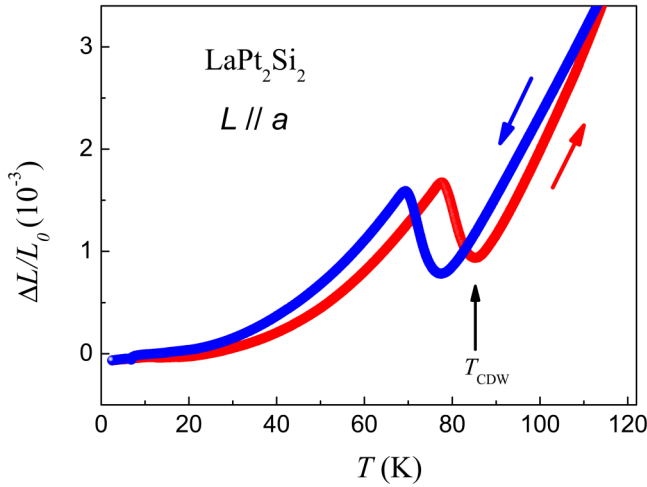


FIG. 2. Temperature dependence of relative thermal expansion ($\Delta L/L_0$) along the a axis for LaPt_2Si_2 for heating and cooling runs as indicated by arrows.

the temperature range 2 K to 120 K for a crystal oriented along the a axis. A hysteresis of approximately 8 K was observed between heating and cooling cycle, which is consistent with the first order nature of the phase transition as seen previously in various measurements. As the temperature decreases the length decreases, which is a common scenario in most of the materials.³⁵ As we further go down in temperature, a minimum is observed at 85 K followed by a maximum at 77 K. The observed behavior in the temperature range from 77 to 85 K is associated with the CDW transition in accord with the resistivity data. Change in relative thermal expansion across the transition is about 0.1%, which matches well with the previous reports where lattice parameters were calculated through temperature-dependent XRD.² The minimal point of the dip in the linear thermal expansion coefficient α_a (shown in Fig. 3) during heating cycle was taken as T_{CDW} . α_a is computed by taking the derivative of the temperature-dependent ΔL vs T data and then dividing it by the length of the sample at room temperature (L_0), i.e.,³⁶

$$\alpha_a = \frac{1}{L_0} \left(\frac{\partial \Delta L}{\partial T} \right)_p. \quad (1)$$

The sizable jump in the value of α_a around T_{CDW} is associated with the structural transition accompanied by a CDW transition. The temperature-dependent thermal expansion coefficient, $\alpha_a(T)$ is fitted to the Debye model excluding the region of the anomaly related to CDW and is shown by solid black line in Fig. 3. The Debye equation used for the fit is given below

$$\alpha_a(T) = \alpha_0 \left(\frac{T}{\theta_D^3} \right) \int_0^{\theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2} dx, \quad (2)$$

where α_0 is a temperature-independent fitting parameter and θ_D is the Debye temperature ($R^2 = 0.98597$). The value of θ_D

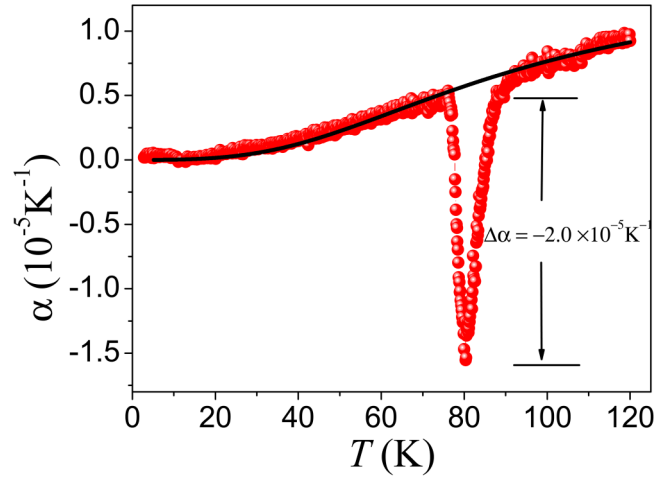


FIG. 3. Linear thermal expansion coefficient, α_a , as a function of temperature for a heating run. The black curve shows the fit to the Debye model given by Eq. (2).

obtained from the fit is 228(1) K, which is close to the value 221.3 (3) K obtained through specific heat data on the same sample, reported earlier.⁹

The jump in the specific heat (ΔC_P) at the CDW transition is related to the change in linear thermal expansion coefficient ($\Delta \alpha_i$, where i stands for the crystallographic axis a , b , or c) at this temperature through the Ehrenfest relation³⁷ given below,

$$\Delta \alpha_i = \frac{1}{V_m} \left(\frac{\Delta C_P}{T_{\text{CDW}}} \right) \left(\frac{dT_{\text{CDW}}}{dP_i} \right), \quad (3)$$

where V_m is the molar volume at room temperature. Putting the value $\Delta C_P = 1.65 \times 10^{-3} \text{ J/mol K}$ (from Ref. 9), $T_{\text{CDW}} = 85.4 \text{ K}$, $V_m = 21.7 \times 10^{-6} \text{ m}^3/\text{mol}$, and $\Delta \alpha_a = -2.0 \times 10^{-5} \text{ K}^{-1}$, we have estimated the uniaxial pressure derivative of the CDW transition temperature, i.e., $\frac{dT_{\text{CDW}}}{dP_a}$ to be -2.26 K/kbar . The Ehrenfest relation in the case of hydrostatic pressure is given by

$$\Delta \alpha = \frac{1}{3V_m} \left(\frac{\Delta C_P}{T_{\text{CDW}}} \right) \left(\frac{dT_{\text{CDW}}}{dP} \right). \quad (4)$$

Using the above relation, we have estimated the derivative of the CDW transition temperature with respect to pressure P , i.e., $\frac{dT_{\text{CDW}}}{dP} = -6.78 \text{ K/kbar}$, which is approximately five times larger than the value obtained through direct transport measurements under hydrostatic pressure, $\frac{dT_{\text{CDW}}}{dP} = -1.27 \text{ K/kbar}$. The difference between the experimentally observed value and the estimated value from specific heat data could be due to the fact that Ehrenfest's theorem assumes isotropic thermal expansion [this is, the origin of the factor 3 in the denominator in Eq. (4)], while experimentally it is seen that the thermal expansion is usually anisotropic. LaPt_2Si_2 shows anisotropic expansion along different axes in the lattice

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parameter data derived from temperature-dependent XRD pattern.² Larger value of $\frac{dT_{CDW}}{dP}$ estimated from Eq. (4) could also be due to underestimation of ΔC_p at T_{CDW} . It is well known that thermal relaxation technique used for specific heat measurement of first order phase transition is not very reliable due to the involvement of latent heat,³⁸ which could give rise to the difference in values of $\frac{dT_{CDW}}{dP}$, measured experimentally and calculated through Eq. (4).

IV. CONCLUSION

We have carried out electrical transport under pressure and thermal expansion experiments on single crystalline LaPt_2Si_2 . The competitive nature of a charge density wave and superconductivity is confirmed through pressure-dependent transport measurements. T_{CDW} decreases with pressure as predicted by the mean field theory and could be understood through the decrease in ω_q with pressure. A sharp decrease in the vicinity of T_{CDW} is seen in α as a function of temperature which is associated with the structural transition accompanied by the CDW transition.

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