Pressure effects on the charge-density-wave phases in 2H-$TaSe_2$

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The transition temperatures from the commensurate to incommensurate phase (T_d) and from the incommensurate to normal phase (T_0) in 2H-$TaSe_2$ have been determined as a function of hydrostatic pressure up to 18 kbar. We found that while T_0 increases only slightly with pressure, T_d falls rapidly as $(1-P/P_c)^{1/2}$ under pressure, extrapolating to a critical pressure P_c of 17 kbar for the complete stabilization of the incommensurate phase. We conclude that the interlayer coupling can not be neglected in discussing the stability of the charge-density-wave state.

INTRODUCTION

Recently the anomalous properties of layered transition-metal dichalcogenides have been the subject of great interest, because of their associated electronic instabilities attributed to charge-density-wave (CDW) formation.[1] The trigonal prismatic coordinated compound 2H-$TaSe_2$ undergoes two intrapolytypic transitions upon cooling as evidenced, e.g., by a sharp resistance kink[2] at ~122 K and a small drop in the resistance[3] at ~90 K. Neutron scattering experiments[4] demonstrated that 2H-$TaSe_2$ is a normal metal above 122 K, and forms a CDW state below 122 K with an incommensurate superlattice which subsequently becomes commensurate below 90 K. The normal to incommensurate phase (N-I) transition at temperature T_0 is second order (or weakly first order at the best),[3,4] whereas the incommensurate to commensurate phase (I-C) transition at temperature T_d is first order.[3,4]

We have measured resistively both the T_d and the T_0 for 2H-$TaSe_2$ as a function of hydrostatic pressure up to 18 kbar. We find that while T_d decreases rapidly with pressure, T_0 increases under pressure with a large quadratic term. The T_d results can be understood qualitatively in terms of the phenomenological Landau theory of CDW states.[4,5] Our pressure data together with those from elastic and neutron scattering[4] measurements also suggest that interlayer coupling is not negligibly small. The present study demonstrates that 2H-$TaSe_2$ is a unique example of a CDW system in which the commensurate phase can be totally inhibited and the formation of the incommensurate CDW state enhanced, by the application of pressure.

EXPERIMENTAL RESULTS

The sample investigated was cut with dimensions of $8\times2\times\sim0.8$ mm^3 (thickness) from a 2H-$TaSe_2$ single crystal grown from the iodine-vapor-transport technique. The electrical resistance (R) along the layers was determined by a standard four-probe ac technique operating at 10 Hz as a function of temperature between 4.2 and 300 K under different compressions up to 18 kbar. Leads were attached to the sample with an ultrasonic soldering iron using indium solder, and indium contacts were lapped over the edges of the sample to make contact with all layers. Both the thermal and pressure cyclings did not generate any breaks in R, typical for a troubled contact in layered-compound study. The modified self-clamp technique[6] was used to provide the hydrostatic pressure environment in a 1:1 fluid mixture of n-pentane and isoamyl alcohol. The pressure was generated by a press and locked by the clamp at room temperature. The pressurized sample together with the clamp was then removed from the press and slowly cooled inside a ^{4}He cryostat. No noticeable shift in either the resistance or transition temperature was detected after the sample was immersed in the pressure medium for two months, indicating that the pressure medium is chemically inert to the sample. A superconducting Pb manometer situated next to the sample was used to measure the pressure at low temperature. Since the pressure change due to cooling usually is small,[7] the quoted pressure is that determined at low temperature (~7 K). The temperature of the sample was determined by an Alumel/Chromel thermocouple[8] at the immediate vicinity of the sample inside the high-pressure medium. All electrical leads were

brought out from the high-pressure environment by Stycast 2850 FT epoxy seals.

At atmospheric pressure, the temperature dependence of R for our $2H$-$TaSe_2$ sample is similar to that previously observed.[3] The N-I phase transition is characterized by a distinct ~1.5% resistance kink at 122 K, and does not exhibit any thermal hysteresis of more than 0.05 K. The I-C phase transition is less conspicuous. Only a small decrease appears in R at 92 K on cooling. However, the thermal hysteresis loop (~3 K), characteristic of a first-order transition, helps to locate the I-C phase transition. The shapes of both transitions are shown in the inserts of Figs. 1 and 2, where T_0 and T_d are also defined. R decreases almost linearly with decreasing temperature above T_0 and quadratically below T_0. The resistance ratio of our sample between 300 and 4.2 K is 170. The application of hydrostatic pressure does not change R more than (0.2–2)% at temperatures below the resistance kink, but slightly suppresses the temperature slope of R above T_0. The maximum reduction of R at 300 K observed is only 4.4% in contrast to ~20% for $2H$-$NbSe_2$.[9]

T_0 was found to be enhanced by hydrostatic pressure with $dT_0/dP = +(3.5 \pm 0.2) \times 10^{-4}$ K bar^{-1} and $d^2T_0/dP^2 = -(7.4 \pm 0.5) \times 10^{-8}$ K bar^{-2} at low pressure, as shown in Fig. 1, where the numbers represented the sequential order of the experimental runs. The presence of a large negative quadratic term in the pressure behavior of T_0 is consistent with the recent observation[3] of the unusually sharp rise in Young's modulus below T_0. On the other hand, T_d is drastically suppressed by hydrostatic pressure, as shown in Fig. 2 where the vertical bar indicates the thermal hysteresis of T_d. No I-C transition was detected for pressure >15 kbar down to 4.2 K. However it should be pointed out that it became increasingly difficult to identify the I-C transition as T_d was suppressed toward lower

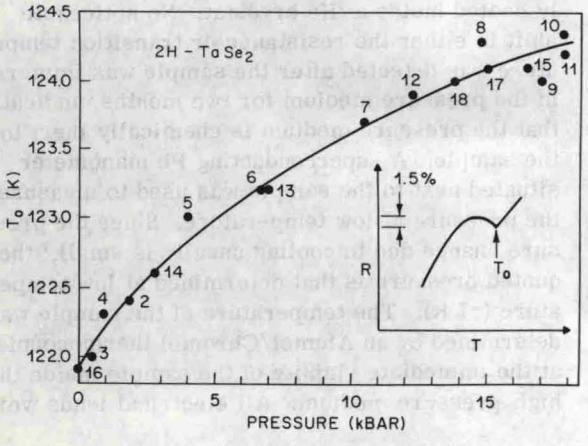

FIG. 1. Pressure dependence of T_0.

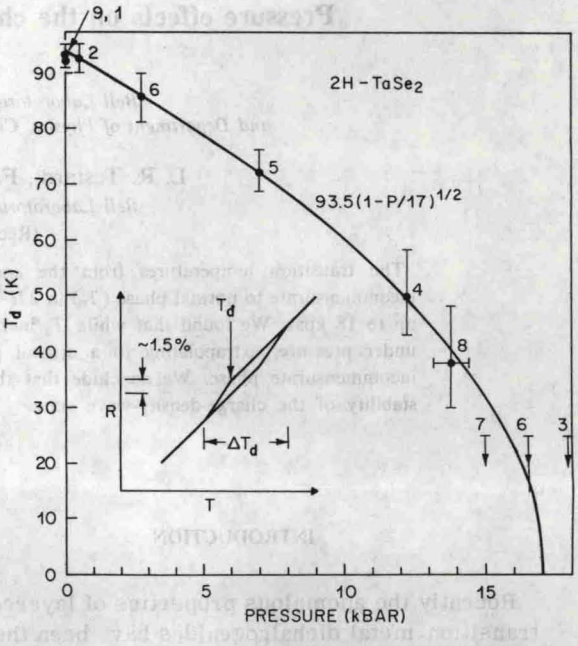

FIG. 2. Pressure dependence of T_d. The circular dot represents T_d defined in the insert, the vertical bar the thermal hysteresis, and the horizontal bar the uncertainty in pressure.

temperature. This is because of the small sample resistance at low temperature which makes the ~1.5% thermal-hysteresis R loop associated with the I-C transition less apparent at low temperature. Therefore an upper limit of 25 K was set for T_d at pressure >15 kbar. T_d fits well the relationship of $T_d(P) = 92.5(1 - P/P_c)^{1/2}$ K with a critical pressure $P_c = 17$ kbar for the complete suppression of the commensurate state, as shown in Fig. 2, although such a pressure behavior is expected for a first-order transition in a metal only as $T \to 0$ K. We found that $dT_d/dP = -(2.7 \pm 0.1) \times 10^{-3}$ K bar^{-1} and $d^2T_d/dP^2 = -(8.0 \pm 0.5) \times 10^{-8}$ K bar^{-2} at atmospheric pressure.

DISCUSSION

It has been shown that a metal will exhibit an electronic instability providing that the electron response function diverges at a wave vector $\vec{q}_0$. This can occur if the Fermi surface of the metal contains parallel pieces or nesting sections,[10,11] or if two-dimensional saddle points[12] in the band structure exist near the Fermi level. A CDW will result when the electron-phonon interaction is strong enough to balance off the Coulomb repulsion, and a spin density wave when the exchange dominates.[11] The characteristic band structure[13] and the strong electron-phonon coupling of these materials make them particularly susceptible to the formation of CDW states. Below T_0, where the