thermal energy is overcome by the energy gain of the CDW states, an incommensurate CDW forms. Further reduction of energy is achieved as the CDW locks into a commensurate geometry at T_d by a slight change of $\vec{q}_0$. In $2H$-$TaSe_2$ the incommensurate state has a $\vec{q}_0 = \frac{1}{3}(1+\delta)\vec{a}^*$ where $\vec{a}^*$ is the reciprocal-lattice vector and δ the temperature-dependent incommensurateness.[4] $|\delta|$ decreases from $\simeq 0.02$ to 0 at T_d.

Phenomenological Landau theories of the CDW states in layer compounds were recently developed by McMillan[5] and Moncton *et al.*[4] The theories correctly describe the sequence of the CDW phase transitions, the negative impurity effects[14] on both T_0 and T_d, and the temperature dependence of the incommensurateness, δ.

The Landau theories predict a decrease in T_d as $|\delta_0|$ (δ at T_0) increases. A decrease in T_d under pressure could be due to an increase in $|\delta_0|$ and/or to a pressure dependence of the Landau parameters that also determine T_d. Diffraction studies to determine δ_0 vs pressure would show if any of the Landau parameters are indeed pressure dependent.

In the $2H$-polytypes, it seems likely that the saddle-point mechanism[12] is the microscopic source of the CDW formation. The effect of pressure on the saddle points near the Fermi level is not immediately evident, however, and thus the change of T_0 with pressure can not be easily predicted.

To determine the effects of interlayer vs intralayer atom spacings on T_0, it is necessary to obtain the uniaxial stress dependences and combine these with the appropriate elastic moduli. The former can be estimated from the behavior of the Young's modulus[3] at T_0 using a thermodynamic treatment.[15] This analysis yields $|dT_0/d\sigma_1| = (0.8 \pm 0.3) \times 10^{-4}$ K bar^{-1} for stress in the basal plane with an undetermined algebraic sign. Combining this result with the present pressure data gives the interlayer stress derivative $dT_0/d\sigma_3 = -(5.1 \pm 1) \times 10^{-4}$ or $-(1.9 \pm 1) \times 10^{-4}$ K bar^{-1} for the "+" and "−" signs, respectively, of $dT_0/d\sigma_1$ above.

In order to determine the strain derivatives, it is necessary to know much of the elastic modulus (stiffness) tensor. From the long-wavelength phonon-dispersion data of Moncton *et al.*[16] one calculates $C_{11} = 23$, $C_{12} = 10.7$, $C_{33} = 5.4$, and $C_{44} = 1.9$, all in unit 10^{11} dyne/cm^2 and with typical uncertainties of ~(10–15)%. The remaining tensor element obtained from the Young's modulus measurement[3] is $|C_{13}| = (7.6+1 \text{ or } 7.6-2) \times 10^{11}$ dyne/cm^2. The algebraic sign cannot be determined from the known data.[17]

Some information on the physically more relevant strain dependences of T_0 can be referred from the above results. These values indicate the importance of interlayer effects in determining T_0. For ideally-two-dimensional behavior,[18] one expects $r \equiv (dT_0/d\epsilon_\perp)/(dT_0/d\epsilon_\parallel) = 0$, where $\epsilon_\perp$ and $\epsilon_\parallel$ are strains perpendicular and parallel to the basal plane. Although there is considerable uncertainty in the calculated results as discussed above, it appears probable that $\frac{1}{3} < |r| < 2$ and, therefore, that interlayer effects are not negligible. Furthermore, for $C_{13} > 0$, $dT_0/d\epsilon_\perp \sim -100$ to -250 K, indicating that, at least to the first order in strain, the interlayer effects would enhance the T_0. A determination of the sign of C_{13} (e.g., from linear compressibility measurements) and of $dT_0/d\sigma_1$ (or $dT_0/d\sigma_3$) would lead to better estimates of the intralayer and interlayer atomic spacing effects.

The importance of interlayer interactions is evident in the band-structure calculations,[13] where the splitting at certain points in the lower d band due to interlayer interactions is equal to the bandwidth. These calculations also showed the sensitivity of these splittings to interlayer separation. It is clear that, if the band splitting changes, the separation of the saddle points from the Fermi level will change. This would establish microscopically, the pressure dependence of T_0 in the saddle-point model.[12]

In conclusion, we have found for the first time that hydrostatic pressure enhances T_0 and suppresses T_d. The rapid reduction of T_d with pressure suggests that the I-C transition sensitively depends on the details of the Fermi surface. The decrease of T_d may be associated with the enhancement of the incommensurateness under pressure or a pressure dependence of the Landau parameters. By analyzing the high-pressure data and the elastic modulus results, the contribution of the interlayer coupling is found to be important in determining the CDW state.

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[17]For $C_{13} > 0$, one finds that hydrostatic pressure leads to a small expansion of the basal plane (and a considerably larger contraction perpendicular to the plane). However, the alternate choice, $C_{13} < 0$, would also indicate relatively unique behavior, since it occurs for very few hexagonal crystals. $C_{13} > 0$ was found for $2H$-$NbSe_2$ and MoS_2 by J. L. Feldman *et al*. [Phys. Rev. B (to be published)].

[18]We assume that $\epsilon_\perp$ occurs mainly in the Van der Waals bonds and that they dominate the calculated values of $dT_0/d\epsilon_\perp$.