

The experimental results show that the optical modes, which are dominated by the intrachain force constants, soften with hydrostatic pressure. In contrast, the long-wavelength acoustical phonons, which mainly probe the interchain force constants, stiffen rapidly. These observations are in general agreement with the ideas of Martin and Lucovsky [5, 6] and Gspan et al. [4] on the nature of the Se-Te system. They predict a transfer of valence charge from bonding orbitals within the chains to bonding states between the chains, both with increasing pressure and with progression towards heavier elements in the group VIb of the Periodic Table. We would like to note that a similar behaviour should be expected for the group Vb elements, where the lattices possess strong covalent bonding within layers and weaker interactions between layers. A study of these materials will be published elsewhere.

With the present pressure data we have studied the homology between Se and Te. We have demonstrated that equivalent optical and acoustical modes in the two materials can be related to each other by a simple transformation involving the mode pressure dependences. The ratio of effective force constants in the two materials with one subjected to a hydrostatic pressure such that their c/a -ratios are identical, has been shown to be approximately equal for most of the zone centre optical and acoustical modes. This indicates that a homological relationship indeed exists between trigonal Se and Te via their respective pressure dependences. We suggest that further experiments on the pressure dependence of zone edge and other phonons should be performed to complete this study.

It was also shown that a high degree of reciprocity exists between the force constants ratios obtained in the independent transformation $\text{Se} \rightarrow \text{Te}$ and $\text{Te} \rightarrow \text{Se}$. This allowed us to predict rough estimates of second-order pressure coefficients (averages between Se and Te) for the zone centre modes considered.

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Appendix A

Assume that the force constant K for a specific mode can be written as a one-term power law in the lattice parameters a and c with exponents x and y :
Before transformation:

$$K_{\text{Te}}(0) = Ac_{\text{Te}}^x(0) a_{\text{Te}}^y(0),$$

$$K_{\text{Se}}(0) = Bc_{\text{Se}}^x(0) a_{\text{Se}}^y(0).$$

After transformation:

$$K_{\text{Te}}(p_{\text{Te}}) = Ac_{\text{Te}}^x(p_{\text{Te}}) a_{\text{Te}}^y(p_{\text{Te}}),$$

$$K_{\text{Se}}(p_{\text{Se}}) = Bc_{\text{Se}}^x(p_{\text{Se}}) a_{\text{Se}}^y(p_{\text{Se}}).$$

This gives the force constant ratios $S_{\text{Te} \rightarrow \text{Se}}$ and $S_{\text{Se} \rightarrow \text{Te}}$

$$S_{\text{Te} \rightarrow \text{Se}} = \frac{K_{\text{Te}}(0)}{K_{\text{Se}}(p_{\text{Se}})} = \frac{A}{B} \left(\frac{c_{\text{Te}}(0)}{c_{\text{Se}}(p_{\text{Se}})} \right)^x \left(\frac{a_{\text{Te}}(0)}{a_{\text{Se}}(p_{\text{Se}})} \right)^y = \frac{A}{B} \left(\frac{a_{\text{Te}}(0)}{a_{\text{Se}}(p_{\text{Se}})} \right)^{x+y},$$

$$S_{\text{Se} \rightarrow \text{Te}} = \frac{K_{\text{Se}}(0)}{K_{\text{Te}}(p_{\text{Te}})} = \frac{B}{A} \left(\frac{c_{\text{Se}}(0)}{c_{\text{Te}}(p_{\text{Te}})} \right)^x \left(\frac{a_{\text{Se}}(0)}{a_{\text{Te}}(p_{\text{Te}})} \right)^y = \frac{B}{A} \left(\frac{a_{\text{Se}}(0)}{a_{\text{Te}}(p_{\text{Te}})} \right)^{x+y}.$$

Note that the condition $(c/a)_B(p_B) = (c/a)_A(0)$ for the transformation has been used to derive the final expressions.

Finally, we arrive at the following condition, using the experimental (and extrapolated) values for the lattice parameter a with and without pressure:

$$S_{\text{Te} \rightarrow \text{Se}} S_{\text{Se} \rightarrow \text{Te}} = \left(\frac{a_{\text{Se}}(0) a_{\text{Te}}(0)}{a_{\text{Se}}(40) a_{\text{Te}}(-35)} \right)^{x+y} = (0.99)^{x+y}.$$

The value in the parenthesis is uncertain to a few per cent due to lack of experimental data. It can therefore be concluded that the reciprocity condition $S_{AB} = S_{BA}^{-1}$ appears to be fulfilled for this case.

References

- [1] W. RICHTER, J. B. RENUCCI, and M. CARDONA, *phys. stat. sol. (b)* **56**, 223 (1973).
- [2] A. v. HIPPEL, *J. chem. Phys.* **16**, 372 (1948).
- [3] P. GROSSE, *Springer Tracts in Modern Physics*, Vol. 48, Ed. G. HÖHLER, Springer-Verlag, Berlin 1969.
- [4] P. GSPAN, R. DROPE, and P. GROSSE, *Verh. DPG* **5**, 286 (1970).
- [5] R. M. MARTIN and G. LUCOVSKY, to be published.
- [6] R. M. MARTIN and G. LUCOVSKY, *Proc. 12th Internat. Conf. Phys. Semicond.*, Stuttgart 1974, Teubner, Stuttgart 1974 (p. 184).
- [7] P. W. BRIDGEMAN, *Proc. Amer. Acad. Arts Sci.* **60**, 303 (1925).
- [8] L. F. VERESHAGIN, S. S. KABELLEING, and B. M. SHULEININ, *Dokl. Akad. Nauk SSSR* **165**, 297 (1965); *Soviet Phys. — Doklady* **10**, 1053 (1966).
- [9] R. M. MARTIN, T. A. FJELDLY, and W. RICHTER, to be published.
- [10] R. I. KUCHER, *Fiz. tverd. Tela* **4**, 2385 (1962); *Soviet Phys. — Solid State* **4**, 1747 (1963).
- [11] M. MOSTOLLER, *J. Phys. Chem. Solids* **31**, 307 (1970).
- [12] G. NILSON and G. NELIN, *Phys. Rev. B* **6**, 3777 (1972).
- [13] P. UNGER and P. CHERIN, in: *The Physics of Selenium and Tellurium*, Ed. W. C. COOPER, Pergamon Press, London/Oxford 1969 (p. 223).
- [14] G. PAPADAKIS, *J. Acoust. Soc. Amer.* **42**, 1045 (1967).
- [15] D. H. CHUNG, D. J. SILVERSMITH, and B. B. CHICK, *Rev. sci. Instrum.* **40**, 718 (1969).
- [16] W. G. CADY, *Piezoelectricity*, Dover, New York 1964 (p. 63).
- [17] J.-L. MALGRANGE, G. QUENTIN, and J.-M. THULLIER, *phys. stat. sol.* **4**, 139 (1964).
- [18] J. MORT, *J. appl. Phys.* **38**, 3114 (1967).
- [19] K. VEDAM, D. L. MILLER, and R. ROY, *J. appl. Phys.* **37**, 3432 (1966).
- [20] P. W. BRIDGEMAN, *Proc. Amer. Acad. Arts Sci.* **74**, 425 (1942).
- [21] D. R. McCANN, L. CARTZ, R. E. SCHMUNK, and Y. D. HORKER, *J. appl. Phys.* **43**, 1432 (1972).
- [22] D. R. McCANN and L. CARTZ, *J. appl. Phys.* **43**, 4473 (1972).
- [23] J. C. JAMIESON and D. B. MCWHAN, *J. chem. Phys.* **43**, 1149 (1965).

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