Pressure Dependence of Elastic Constants in Se and Te

dependence for the two lattices [13]. This, therefore, leaves only one extra degree of freedom, and we have arbitrarily chosen to consider the c/a-ratio, which is different in the two materials: we can produce $(c/a)_A$ of species A by pressurizing species B and vice-versa. Thus, we have a two-step transformation which consists of subjecting B to a pressure p_B until $(c/a)_B(p_B) = (c/a)_A(0)$, and then secondly executing the mass and unit cell scaling. When this transformation is performed on the lattice modes of species B, the comparison with species A gives valuable information about the corresponding force constants in the two materials. Our aim is, with the present data on zone centre phonons, to demonstrate the possible existence of a homological relationship between the two elements. Of course, the transformation can be carried out both ways, either $A \rightarrow B$ or $B \rightarrow A$, and we shall see that this leads to interesting conclusions about the reciprocity of the scaling of the force constants. In addition, a simplified approach allows us also to estimate magnitudes for higher order pressure coefficients for the lattice modes.

2. Experimental

The various sound velocities and their pressure dependence were measured with a standard ultrasonic pulse-echo overlap technique [14, 15]. The experimental set-up was built around a Matec 6000 rf pulse generator. The frequencies used were 20 to 30 MHz; and the quartz transducers were bonded to the samples with Nonaq stop-cock grease or solidified phenylsalycilate ("salol"). The latter proved a good and reliable bond that normally did not break when applying pressure. Moreover, in check runs with grease bonds, no observable distortions that could be attributed to the use of solid bonds were detected in the data.

The single crystal samples of Se and Te were prepared as plates ranging in thickness from 2.5 to 5 mm with faces perpendicular to the X-axis (only Te) and the Y- and Z-axis³) (both Se and Te). The samples were X-ray oriented to $\pm 1^{\circ}$. The surfaces were carefully lapped in a lapping jig with a light-weight (hollow) aluminium piston.

The hydrostatic pressure was achieved in a steel bomb furnished with a coaxial electrical feed-through. Silicone oil was used as the pressure transmitting fluid, and the system had a capability of 7 kbar. A standard manganin resistive cell served as the pressure gauge.

3. Results

The measured pressure dependence of effective elastic constants are shown in Fig. 1 and 2, not corrected for volume and length changes. These corrections have to be applied as the pulse-echo method measures only the transit time of a pulse through the sample. For a determination of velocities as a function of pressure one therefore needs the dependence of the sample length on pressure, which is determined through the linear compressibilities. To calculate the elastic constants one has in addition then to correct for the density changes, given by the volume compressibility. The compressibilities can be calculated from a complete set of zero pressure elastic constants [16]. The elastic constant C_{13} , which can only be determined by measurements with wave-vector directions between

³) The Z-direction corresponds to the trigonal axis; X is the twofold axis (in the basal plane) and Y is perpendicular to both X and Z (i.e., Y is also in the basal plane).

T. A. FJELDLY and W. RICHTER





Fig. 1. Relative change in the effective elastic constants with hydrostatic pressure in Te; uncorrected for length and volume changes

Fig. 2. Relative change in the effective elastic constants with hydrostatic pressure in Se; uncorrected for length and volume changes

the c-axis and the basal plane, was not measured here. We therefore took the compressibilities from the results of X-ray measurements under hydrostatic pressure, made by various authors. For Te the compressibilities quoted [7] are compatible with the value of C_{13} given by Malgrange et al. [17]. For Se large inconsistencies exist between the elastic constants [18, 19], linear compressibilities [8, 22], and volume compressibilities [20, 21]. This is probably due to the fact that none of these compressibility measurements has been performed on single crystalline material and in a true hydrostatic environment, conditions necessary for such an anisotropic and soft material like Se. Therefore the corrections performed on the Se data are somewhat uncertain. The corrected logarithmic pressure derivatives for the effective elastic constants are shown in Table 1. From the six independent hydrostatic pressure coefficients, we have information on five in both Se and Te; with three redundancies in the case of Te for checks on internal consistency. The sixth coefficient, involving the elastic constant C_{13} , was not determined here. We also obtained absolute values of the elastic constants, and these are compared with published data in Table 1. Our data on Te are in excellent agreement with those of Malgrange et al. [17]. Note that the effective "mode" elastic constants listed for the X- and Y-direction by Malgrange et al. were computed from their list of elastic constants using the expressions

$$C_{2,3} = \frac{1}{2} \left(C_{66} + C_{44} \right) \pm \left(\frac{1}{4} \left(C_{66} - C_{44} \right)^2 + C_{14}^2 \right)^{1/2} \tag{1}$$

for the two mixed transverse modes in the X-direction and

$$C_{4,5} = \frac{1}{2} \left(C_{11} + C_{44} \right) \pm \left(\frac{1}{4} \left(C_{11} - C_{44} \right)^2 + C_{14}^2 \right)^{1/2}$$
(2)