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TECHNICAL NOTE

The high pressure compressibility and Grüneisen parameter of strontium titanate*

AT TEMPERATURES above 108°K, $SrTiO_3$ is a paraelectric material crystallizing in the cubic perovskite structure. We have measured the compressibility of $SrTiO_3$ and fitted the data to the Murnaghan equation of state. In addition, the Grüneisen parameter calculated from our high pressure compressibility data is compared to the Grüneisen parameter calculated from the zero pressure values of the compressibility, thermal expansion, heat capacity at constant volume, and molar volume.

Data were obtained by means of a diamond anvil high-pressure X-ray diffraction camera described elsewhere[1]. Pressures were determined by observing the shift of the diffraction lines of a 'marker', a material with known compressibility, mixed with the $SrTiO_3$. In this work, CsBr, Al, and V were used as 'markers'. For CsBr, Bridgman's [2] compressibility data were used; for Al and V, the data of Rice *et al.*[3] were used. The $SrTiO_3$ was prepared at this laboratory and was at least 99·99 per cent pure. Samples were prepared for loading in the diamond anvil high-pressure cell by first mixing the $SrTiO_3$ with the appropriate 'marker' and then pressing the powder to about 8 kbar. A small chip from the resultant wafer was used as the high-pressure sample.

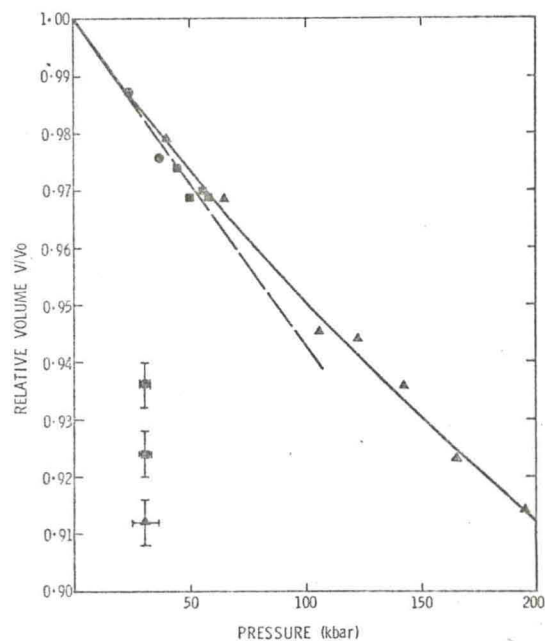In Fig. 1, the relative volume $V/V_0 =$

Fig. 1. Relative volume vs. pressure for $SrTiO_3$. Three 'markers', CsBr (●), Al (■), and V (▲), were used to determine pressure. The error bars at the bottom of the figure indicate the uncertainty for each of the 'markers.'

a^3/a_0^3 is plotted vs. pressure where V_0 and a_0 are the unit cell volume and lattice parameter, respectively, at atmospheric pressure. At 298°K and 1 bar, the lattice parameter, a_0, of $SrTiO_3$ is 3·9051 Å[4]. The dashed line in Fig. 1 is an extrapolation of the initial compressibility of $SrTiO_3$ determined from the elastic constants[5] and the solid curve was obtained by a least squares fit of our data to the Murnaghan equation of state[6],

$$P = \frac{B_0}{B_0'}\left\{\left(\frac{V_0}{V}\right)^{B_0'} - 1\right\},$$

where the initial bulk modulus is

$$B_0 = \left\{ -V\left(\frac{\partial P}{\partial V}\right)_T \right\}_{P=0},$$

and the corresponding pressure derivative

$$B_0' = \left\{ \left(\frac{\partial B}{\partial P}\right)_T \right\}_{P=0}.$$

The elastic constants of Bell and Rupprecht [5] were used to calculate $B_0 = 1 \cdot 76 \times 10^3$ kbar and the best fit to our data was obtained with $B_0' = 4 \cdot 4$.

One can determine the Grüneisen parameter for $SrTiO_3$ from the Grüneisen relation[7]

$$\gamma = \frac{\alpha V_m}{\beta C_v},$$

where α is the volume thermal expansion, V_m is the molar volume, β is the compressibility, and C_r is the specific heat at constant volume. At room temperature and atmospheric pressure, the values of the various parameters are $\alpha = 2 \cdot 6 \times 10^{-5}$°K[8], $\beta = 5 \cdot 67 \times 10^{-13}$ cm^2/dyne[5], $C_r = 20 \cdot 7$ cal/mole-°K[9] and $V_m = 35 \cdot 7$ cm^3/mole; using these values, one calculates $\gamma = 1 \cdot 89$. The B_0' obtained from the least squares fitted Murnaghan equation can be used to calculate the Grüneisen parameter by an independent

method; Anderson[10] has shown that

$$\gamma = \frac{B_0' - 1}{2}.$$

As mentioned previously, the data was best fit with $B_0' = 4 \cdot 4$, and thus $\gamma = 1 \cdot 7$, in reasonable agreement with the value calculated above.

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REFERENCES

1. LYNCH R. W., *J. chem. Phys.* **47**, 5180 (1967).
2. BRIDGMAN P. W., *Proc. Am. Acad. Arts. Sci.* **76**, 1 (1945).
3. RICE M. H., McQUEEN R. G. and WALSH J. M., *Solid St. Phys.* **6**, 1 (1965).
4. WYCOFF R. W. G., *Crystal Structures*, p. 394. Wiley, New York (1964).
5. BELL R. O. and RUPPRECHT G., *Phys. Rev.* **129**, 90 (1963).
6. MURNAGHAN F. D., *Proc. natn. Acad. Sci. U.S.A.* **30**, 244 (1944).
7. KITTEL C., *Introduction to Solid State Physics*, p. 154. Wiley, New York (1956).
8. KRIKORIAN O. H., University of California Radiation Laboratory Report UCRL-6132 (1960).
9. COUGHLIN J. P. and ORR R. L., *J. Am. chem. Soc.* **75**, 530 (1953).
10. ANDERSON O. L., *Phys. Rev.* **144**, 553 (1966). Sandia Laboratories.