J. Phys. Chem. Solids Pergamon Press 1970. Vol. 31, pp. 573–574. Printed in Great Britain.

L. R. Edwards

TECHNICAL NOTE

The high pressure compressibility and Grüneisen parameter of strontium titanate*

(Received 27 May 1969; in revised form 8 August 1969)

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.

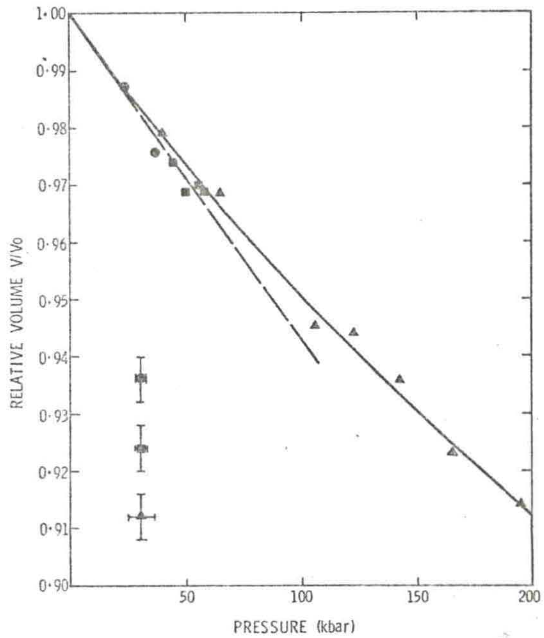

Fig. 1. Relative volume vs. pressure for $SrTiO_3$. Three 'markers', CsBr (●), Al (■), and V (▲), were used to determine pressure. The error bars at the bottom of the figure indicate the uncertainty for each of the 'markers.'

In Fig. 1, the relative volume $V/V_0 = a^3/a_0^3$ 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],

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

*This work was supported by the U.S. Atomic Energy Commission.