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PRESSURE DEPENDENCE OF COMPRESSION FOR SOLIDS USING LOW PRESSURE ULTRASONIC DATA

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Calculations of compression at various pressures have been done in TlBr, single crystal spinel (MgO. 2.6 Al_2O_3), fused quartz, alpha iron and MnSb using the polynomial equations and the Murnaghan logarithmic equation. Comparison, whereever possible, have been made with the experimental results. It is found that the logarithmic equation holds well for explaining the pressure dependence of compression even at high pressures. In the evaluation of compression, all the parameters required were calculated from low pressure ultrasonic data.

Introduction

Generally in order to measure the compression in solids three types of experimental techniques are used: *1*) measurement of lattice constants at different pressures, *2*) measurement of volume change, and *3*) the use of shock waves. However, it was found that the methods reliable at low pressures are not quite suitable at high pressures. Measurements of the ultrasonic velocity, the bulk modulus and their derivatives can be done with great precision but their pressures range is limited. However, the ultrasonic data at low pressures have been succesfully used to evaluate compression at high pressures [1]. The agreement between the calculated and experimental compression values was found to be quite satisfactory for some of the compressible and incompressible solids.

In the present paper, we have calculated and compared the compression values with the experimental ones for the solids TlBr, single crystal spinel (MgO.2.6Al_2O_3), fused quartz, alpha iron and MnSb.

Procedure

The method for calculating the compression involves mainly the assumption that the bulk modulus is a linear function of pressure and that the second and higher derivatives of the bulk modulus are negligibly small. Expanding the volume V in MacLaurin's series

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in powers of P and expressing the derivatives of V in terms of the derivatives of B it is possible to arrive at the following polynomial equations [1]:

The quartic polynomial:

$$(V/V_0) = 1-(P/B_0)+m(P/B_0)^2-n(P/B_0)^3+q(P/B_0)^4 \tag{1}$$

and the cubic polynomial:

$$(V/V_0) = 1-(P/B_0)+m(P/B_0)^2-n(P/B_0)^3 \tag{2}$$

where,

$$m = \frac{1}{2}(1+B_0')$$

$$n = \frac{1}{6}(1+3B_0'+2B_0'^2)$$

and

$$q = \frac{1}{24}(1+6B_0'+11B_0'^2+6B_0'^3).$$

The primes indicate (d/dP).

In 1944 Murnaghan [2] proposed a formula for evaluating compression at various pressures:

$$P = (B_0/B_0')[(V_0/V)^{B_0'}-1]. \tag{3}$$

This is commonly known as the: Murnaghan logarithmic equation which can be further written as:

$$\ln(V_0/V) = (1/B_0')\ln[B_0'(P/B_0)+1]. \tag{4}$$

This equation has been successful in describing the pressure variation of compression in some solids. However, equation (4) describes the compression better than the polynomials at high pressures, but at modest pressures the polynomials do agree very well with the Murnaghan's exponential equation and the experimental results.

Results and conclusions

In view of the success of the equations (1) and (4) in predicting compression for some compounds, it is proposed to check their validity in TlBr, single crystal spinel, quartz, alpha iron and MnSb. The necessary data for the evaluation of m, n and q have been taken from the literature [3–7].

Figures 1 and 2 show the pressure variation of compression for TlBr as estimated from equations (1), (2) and (4). The solid line in figure 1 is the result of calculations with equation (4) using the value of B_0' evaluated from equation (27) of reference [1]. The dashed line is due to the value of B_0' according to the relation given by Dugdale and MacDonald [8]:

$$B_0' = 2\gamma+1.$$

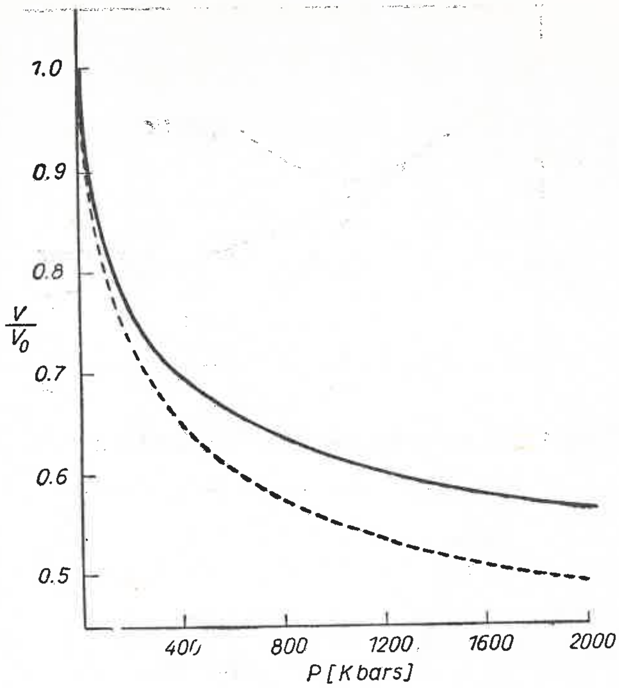

Fig. 1. Compression for TlBr. See text for solid and dashed lines

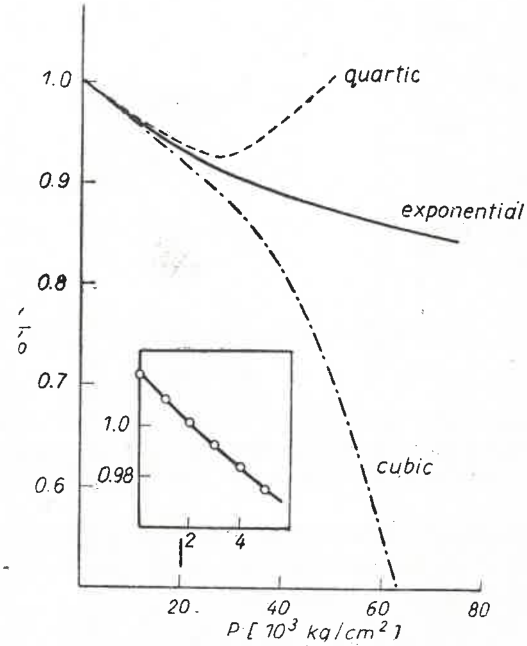

Fig. 2. Compression for TlBr. Comparison of logarithmic and polynomial equations. Inset: A comparison between the polynomials (solid line) and V/V_0 calculated from Eq. 17 of reference [3] in the experimental range

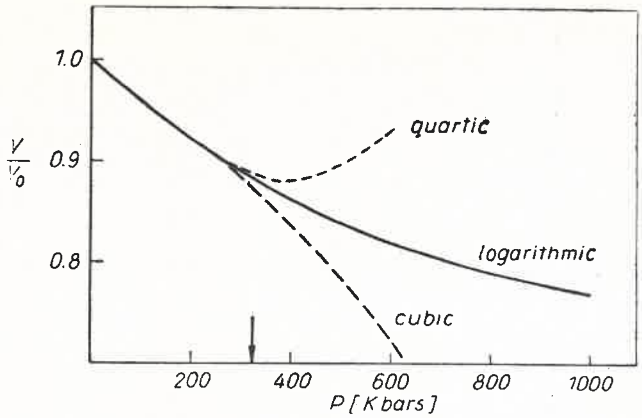

Fig. 3. Compression for single crystal spinel, MgO. 2.6 Al_2O_3.

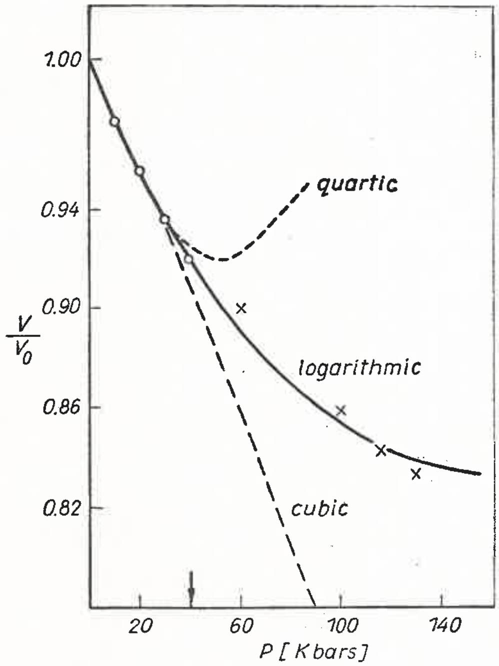

Fig. 4. Compression for fused quartz; Experimental points: ○ — P. W. Bridgman, *Collected experimental papers*, Vol. 1–7, Harward University Press (1964); *Proc. Amer. Acad. Sci.*, **76**, 55 (1948). × — Schock wave data: J. Wackerle, *J. Appl. Phys.*, **33**, 922 (1962).

Figure (2) shows a comparison between the logarithmic equation and the polynomials. The inset shows a comparison between the polynomials (solid line) and the values of compression calculated according to the equation:

$$(V/V_0) = 1 - EP + FP^2$$

where E and F are constants determined experimentally [3].

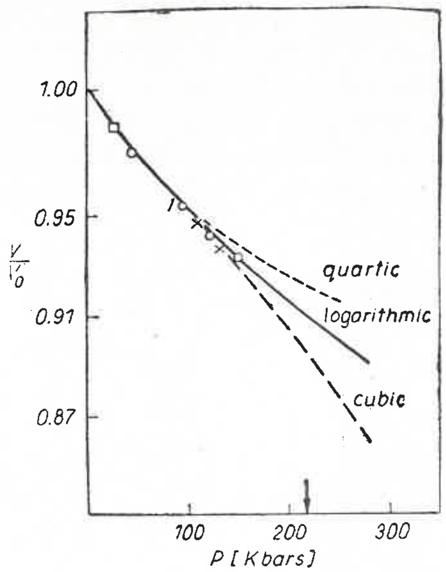

Fig. 5. Compression for alpha iron; Experimental points: ○ — T. Takahashi, and W. A., Basset, *Science*, **145**, 483 (1964). □ — P. W. Bridgman, *Proc. Amer. Acad. Sci.* **76**, 55 (1948). × — D. Bancroft, E. L. Peterson, S. Minshall, *J. Appl. Phys.* **27**, 291 (1956)

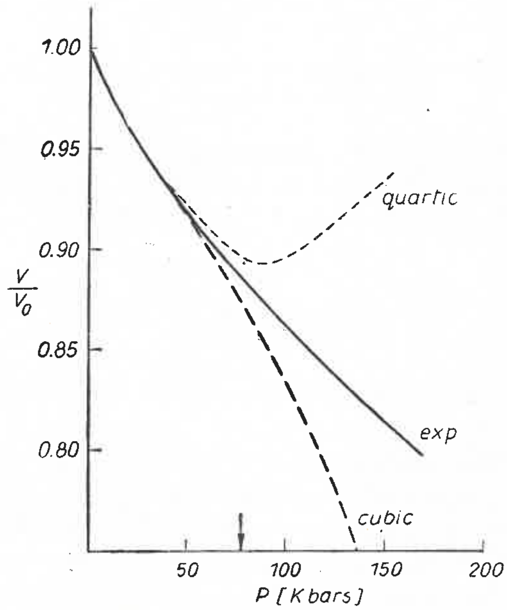

Fig. 6. Pressure variation of compression of MnSb

The values of compression calculated from equations (1), (2) and (4) for single crystal spinel, fused quartz and alpha iron are shown in figures 3 to 5. Experimental points have also been plotted for quartz and alpha iron. The pressure variation of compression in MnSb [7] corresponds to the Murnaghan equation with $B_0 = 470$ Kbars and $B_0' = 4$ for the best fit. The values of m, n and q can thus be evaluated which, in turn, are used to calculate the pressure dependence of compression by quartic and cubic polynomials. The results are shown in Figure 6.

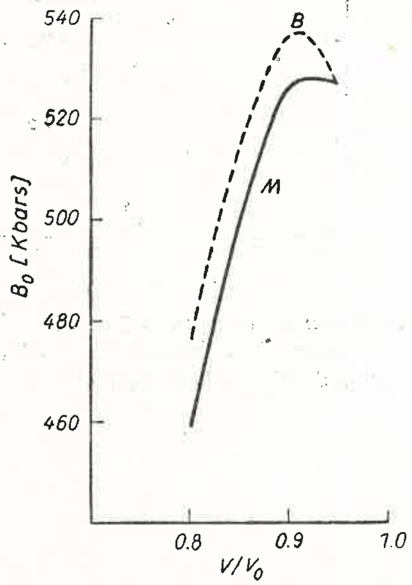

Fig. 7. Variation of B_0 with compression for MnSb: ——— calculated from Murnaghan's equation, — — — calculated from Birch's equation of state

That the logaritmic equation gives the best result in all the solids, suggests that the polynomials depart noticeably from the real value at somewhat higher pressures. It turns out that the pressure P' where the cubic is barely within 1% of the logatrihmic curve, is calculated by

$$P' = \frac{1}{2}\frac{m}{n}B_0.$$

The value of P' is important to the experimenters who fit an arbitrary cubic curve to raw compression data, because otherwise the curve at low pressures will give an incorrect value of the compressibility. The calculated values of P' is shown in the figures by an arrow. The values of m, n and q used in the evaluation are shown in Table I.

We now make a comparison of the logarithmic equation with Birch's equation of state [9] for the special case $B_0' = 4$ which is true for the case of MnSb. The values of P/B_0 for various values of V/V_0 have been tabled [1]. As the values of P can be determined from figure 2 of reference [7], the variation of B_0 with V/V_0 can now be evaluated and is shown in

TABLE I

Parameters used in the evaluation of compression

Solid	m	n	q
TlBr	4.21	22.28	129.50
Single Crystal spinel	2.59	8.11	27.54
Alpha iron	3.10	11.80	48.83
Fused quartz	3.58	15.90	77.40
MnSb	2.50	7.50	24.40

Figure 7. The use of logarithmic and Birch's equation of state both give a variation of B_0 with compression quite far from the used value of 470 Kbars.

In all the cases the superiority of Murnaghan's equation over the cubic and quartic polynomials is well demonstrated throughout the pressure range. However, the polynomials are quite accurate in predicting the compression at modest pressures and agree with the logarithmic equation up to pressure P'. They are also useful for incompressible solids up to pressures of 300 Kbars. The main advantage of the method is that the compression at high pressures are evaluated without using any arbitrary parameters or curve-fitting.

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