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Extrapolation Formula for Finding the Volume of Solids at High Pressures

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A formula is proposed for extrapolating from data taken at low or moderate pressures to the high pressures that exist in the interior of the earth and planets. The formula, which predicts the curve of reduced volume v/v_0 versus reduced pressure $P \equiv p/K_0$, follows from integration of the following assumed expression for the pressure derivative of the bulk modulus $K \equiv -v\, dp/dv$

$$d(K/K_0)/dP = m + \frac{a^2(K_0' - m)}{(P + a)^2}$$

When $m = K_0'$, the formula reduces to the well-known Murnaghan relation, which is itself remarkably successful. In general, there is an improvement on the Murnaghan relation because the above expression allows the derivative to change from its initial value K_0' to a more realistic value m as $P \to \infty$. The Keane equation, $d(K/K_0)/dP = m + (K_0' - m)/(K/K_0)$, has this same property, but with the disadvantage of behaving unreasonably if $K_0' < 0$. To apply our formula, K_0' is determined from low-pressure ultrasonic data (0 to 6 kb), m is fixed at some reasonable value, and the remaining parameter is then determined by trial and error to fit the high-pressure data that are available. Rough estimates of the initial value of the second pressure derivative of the bulk modulus can be obtained in this way. As examples, the formula is fitted to experimental data that are already in the literature on aluminum oxide, α-quartz, magnesium, potassium, sodium, and lead.

INTRODUCTION

A few years ago, *Anderson* [1966] emphasized that the extrapolation formula of *Murnaghan* [1944], which is based on the assumption of a linear pressure dependence of the bulk modulus, is remarkably successful in predicting the volume of a solid at high pressures. More recently, *Anderson* [1968] pointed to the need for an improved formula and recommended the Keane equation [*Keane*, 1954]. In the present paper, we give a formula that has the advantage of the Keane equation while incorporating an additional parameter for increased flexibility.

The Keane equation can be obtained by integration from

$$\frac{d(K/K_0)}{dP} = m + \frac{K_0' - m}{K/K_0} \qquad (1)$$

where $P = p/K_0$, p being the pressure, K is the bulk modulus, K_0 its value at zero pressure, K_0' its first pressure derivative evaluated at zero pressure, and m the value of the first pressure derivative in the limit as $K \to \infty$. Anderson's recommendation is to determine K_0 and K_0' from ultrasonic data taken at low pressures, and m from shock wave data at higher pressures. This procedure gives an excellent fit to the available experimental data. Whenever K_0' and m are both positive, the extrapolation behaves reasonably on the entire range $P > 0$. However, if K_0' is negative, the Keane equation predicts unreasonable behavior in that it forces K to go to zero at some positive pressure.

There is a class of materials, mainly certain glasses, where K_0' is negative, although dK/dp becomes positive and behaves normally at sufficiently high pressures. This class includes vitreous silica [McSkimin as cited by *Anderson*, 1961], obsidian [*Manghnani et al.*, 1968], germania glass [*Soga*, 1969], and vycor [*Manghnani and Benzing*, 1969]. The previous extrapolation formulas do not handle this class at all.

The present proposal is to take