Isothermal equations of state for lithium fluoride

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The change in length of 1-m-long LiF single crystal has been determined as a function of hydrostatic pressure up to 7 kbar over the temperature range 28–41°C. The length change has been measured to an accuracy of less than 500 A by using a Fabry-Perot type He-Ne laser interferometer, and under a temperature-controlled environment with temperature variations less than 0.002°C. Several isothermal equations of state, together with those derived from the Born model of ionic solids, have been used in analyzing the pressure-volume data. The isothermal bulk modulus B_o and its pressure derivative B'_o at atmospheric pressure and 28.83 ± 0.05°C obtained from the two-parameter (B_o and B'_o) equations of state are $B_o = 664.5 \pm 0.5$ kbar and $B'_o = 5.40 \pm 0.18$, respectively. The present results differ considerably from the static measurements of Bridgman and also of Vaidya and Kennedy, but are in excellent agreement with the values obtained by ultrasonic measurements. Using the two-parameter equations of state, the pressure volume data is extrapolated to ~5 Mbar in order to compare with the shock wave data and to examine the differences between the various equations of state, which are hardly distinguishable in the low-pressure region. Although the present V/V_o measurements are sufficiently accurate to obtain accurate values of B''_o, the present pressure measurements are not (although we believe they are as accurate as is possible at the present time).

PACS numbers: 64.30.+t, 65.50.+m, 65.70.+y

INTRODUCTION

Several equations of state have been used in the literature[1] to fit the pressure-volume-temperature data of solids. Most of these equations are phenomenological. A detailed treatment and discrimination between these equations has been provided by MacDonald and his co-workers.[2–4] An excellent review of these equations has also been given by Knopoff.[5]

Let V denote the volume of a specimen and P the pressure applied to it, at some constant temperature T. Then, an isothermal bulk modulus B is defined as $B \equiv -V(\partial P/\partial V)_T$ which at a given reference pressure P_0 shall be $B_0 = -V_0(\partial P/\partial V)_{P=P_0}$. The first- and second-order pressure derivative of the bulk modulus evaluated at $P = P_0$ shall be denoted by B'_0 and B''_0, respectively. For convenience, we shall introduce the following notations $p \equiv P - P_0$, $\eta \equiv B'_0$, $\psi \equiv B_0 B''_0$, $z \equiv p/B_0$, and $x \equiv V_0/V$. Note that η, ψ, z, and x are all dimensionless quantities. P_0 is assumed to be 1 bar in this paper.

The two- and three-parameter phenomenological equations of state[6–10] discussed in this paper are listed in Table I. Also included in this table are two lattice equations of state based on the Born Model. As it has been widely investigated in the literature[11,12] only the barest outline will be given here. In deriving those equations of state, the van der Waals contribution to the lattice energy for LiF being small has been ignored. It is considered to be a static lattice and the repulsive potential chosen is A/r^n for the Born-Mie potential and $\lambda \exp(-r/\rho)$ for the Born-Mayer potential where (A, n) and (λ, ρ) are the repulsive parameters.

When the pressure-volume data on the basis of the two-parameter equations of state are extrapolated to a high-pressure region and then compared with shock wave data, the agreement is not always good. The improvement that can be made by using a three-parameter equation of state has been recently investigated by Anderson[13] on the basis of Keane's equation of state. Barsh and Chang[14] on the basis of their ultrasonic data of cesium halides conclude that the three-parameter equation of Birch is superior to Keane's equation.

In other words, there is considerable need and interest for the higher-pressure derivative B''_0. How-

TABLE I. Various equations of state.

Equation	Acronym	Form
First-order Murnaghan	ME$_1$	$z = \eta^{-1}[x^{\eta} - 1]$
Second-order Murnaghan	ME$_2$ ($\eta^2 \geq 2\psi$)	$z = (2x^{(\eta^2-2\psi)^{1/2}} - 1)/[(\eta^2 - 2\psi)^{1/2}(x^{(\eta^2-2\psi)^{1/2}} + 1) - \eta(x^{(\eta^2-2\psi)^{1/2}} - 1)]$
Keane	KE ($-\eta^2 < \psi < 0$)	$z = [\eta^3/(\eta^2+\psi)^2](x^{(\eta^2+\psi)/\eta} - 1) - [\psi/(\eta^2+\psi)]\ln x$
First-order Birch	BE$_1$	$z = (3/2)(x^{7/3} - x^{5/3})[1 + (3/4)(\eta - 4)(x^{2/3} - 1)]$
Second-order Birch	BE$_2$	$z = (3/2)(x^{7/3} - x^{5/3})\{1 + (3/4)(\eta - 4)(x^{2/3} - 1) + (1/24)[143 + 9\eta)(\eta - 7) + 9\psi](x^{2/3} - 1)^2\}$
Grover Getting Kennedy	GGKE	$B_T = B_0^T \exp[\eta(1 - x^{-1})]$
Born-Mie	BME	$z = 3(x^{n+3/3} - x^{4/3})/(n - 1)$
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The two- and three-parameter phenomenological equations of state[6–10] discussed in this paper are listed in Table I. Also included in this table are two lattice equations of state based on the Born Model. As it has been widely investigated in the literature[11,12] only the barest outline will be given here. In deriving those equations of state, the van der Waals contribution to the lattice energy for LiF being small has been ignored. It is considered to be a static lattice and the repulsive potential chosen is A/r^n for the Born-Mie potential and $\lambda \exp(-r/\rho)$ for the Born-Mayer potential where (A, n) and (λ, ρ) are the repulsive parameters.

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TABLE III. Isothermal bulk modulus and its pressure derivative of LiF.

Source	Temp. (°C)	B_0 (kbar)	B_0'
Present work	28.83	664.5	5.40 [a]
Miller and Smith (Ref. 18)	27	664	5.24 [b]
Haussühl (Ref. 19)	22	665	
Vaidya and Kennedy (Ref. 17)	Room	627.8	6.82
Bridgman (Ref. 17)	Room	621	9.15

[a] An average value of the two-parameter equations in Table II.
[b] Corrected to an isothermal value.

Liquid hexane is used as a pressure fluid and is transmitted through a pressure tubing (0.475-cm o.d. and 0.063-cm i.d.) to the pressure vessel. Connected in series with the length measurement pressure vessel is another pressure vessel where manganin wire, the pressure sensor, is kept. The technique used to calibrate the manganin gauge is described in detail elsewhere.[22]

The lenght measurements were made at an interval of 500 bar up to a maximum of 7 kbar at each temperature. The experiment at each temperature was carried out twice to check for the reproducibility of the data. Inasmuch as the linear compressibility for LiF is isotropic, the length measurement data is transformed to volume measurements using the relation $V/V_0 = (l/l_0)^3$. For equation-of-state measurements, one is never concerned with V_0 itself but only the ratio V/V_0. Consequently, it is neither necessary to measure the specimen diameter nor to have a uniform diameter.

RESULTS

All the equations of state listed in Table I have been used to fit the measured pressure-volume data by the least-squares method. As indicated in Table II, the two-parameter (B_0 and B_0') equations lead to satisfactory results. ME_1 is the only equation of state in that list for which B_0'' equals zero. The expressions for BE_1 and GGKE do not explicitly contain the parameter B_0''. However, this does not imply that it is identically zero for those equations. The appropriate expression for B_0'' in the case of BE_1 is given by

$$9B_0B_0'' = -[143 + 9B_0'(B_0' - 7)] \tag{1}$$

and is obtained by setting the third term in the second-order Birch equation BE_2 identically equal to zero. Successive differentiation of the GGKE equation with respect to pressure and taking the limit as $P \rightarrow P_0$ yields

$$B_0B_0'' = -B_0'^2 \tag{2}$$

from which one can then calculate B_0''. These calculated values are tabulated also in Table II. The fit to the three-parameter equations has been found to be poor resulting in an unexpected high value of $|B_0''|$. The bulk modulus data measured by other authors, together with the present work at 28.83 °C are also recorded in Table III for the sake of comparison. Present measurements of B_0 and B_0' agree rather well with those obtained by ultrasonic techniques, and the agreement is poor when compared with the earlier values obtained from the static compression method. Thermal properties of LiF, measured between 28.8 and 40.9 °C, are shown in Table IV. Noting the small temperature range considered, too much credit should not be given to them.

TABLE IV. Thermal properties of LiF.[a]

Volume thermal expansion coeff. β (10^{-4}/°C)	$\left.\frac{\partial\beta}{\partial T}\right\|_P$ (10^{-7}/°C^2)	$\left.\frac{\partial B_0}{\partial T}\right\|_P$ (kbar/°C)	$\left.\frac{\partial B_0'}{\partial T}\right\|_P$ (10^{-2}/°C)
1.043 ± 0.003	1.62 ± 0.66	−0.38 ± 0.03	−1.6 ± 2.2

[a] Evaluated at $T = 28.8$ °C.

TABLE V. Output data at $T = (28.83 \pm 0.05)$ °C.

Equation used	B_0 (kbar)	Repulsive parameter[a]	B_0'	B_0'' (kbar^{-1})
Born-Mie	664.89 ± 0.22	8.92 ± 0.24	5.31	−0.00796
Born-Mayer	664.50 ± 0.23	11.43 ± 0.26	5.41	−0.0102

[a] The repulsive parameter means n for the Born-Mie potential and r_0/ρ for the Born-Mayer potential.

Table V indicates the parameter B_0 and the repulsive parameter obtained by fitting the experimental data to the lattice equations of state mentioned in Table I. The parameter B_0' and B_0'' were calculated[23] using the expressions

$$B_0' = \tfrac{1}{3}(n + 7), \tag{3}$$

$$B_0B_0'' = -\tfrac{4}{9}(3B_0' - 4) \tag{4}$$

which are appropriate for the Born-Mie potential and

$$B_0' = 2 + \frac{\{(r_0/\rho)[(r_0/\rho) - 3]\}}{3[(r_0/\rho) - 2]}, \tag{5}$$

$$B_0B_0'' = -(B_0' + 1)(B_0' + 2) + \frac{\{(r_0/\rho)^3 + 12(r_0/\rho)^2 + 52(r_0/\rho) - 200\}}{9(r_0/\rho) - 2} \tag{6}$$

for the Born-Mayer potential. As can be seen, the parameters B_0 and B_0' obtained from the lattice equations of state agree remarkably well with those obtained by using the two-parameter phenomenological equations of state.

DISCUSSION

As shown in Tables III and V the two-parameter equations yield virtually identical results for B_0 and B_0'. However, when one resorts to three-parameter equations, the values obtained for $|B_0''|$ are consistently too high. The ultrasonic measurements of $B(P)$ versus P on LiF show no signs of curvature[18] up to 8 kbar. If the error in B_0' from ultrasonic measurements is attributed entirely to curvature, then one estimates that $|B_0''|$ is ≤ 0.03. However, one can possibly conclude that the sign of B_0'' is negative. Even though

TABLE VI. Bulk modulus and its pressure derivatives based on the assumption that the nonlinear pressure variation with the change in resistance of the manganin gauge is cubic.

Equation used	B_0 (kbar)	B'_0	$B''_0)$[a] $(\text{kbar})^{-1}$	Temperature (°C)
ME_1	664.50 ± 0.18	5.34 ± 0.07	0.00 ± 0.00	28.83
ME_2	663.44 ± 0.30	6.36 ± 0.27	-0.32 ± 0.10	28.83
GGKE	664.49 ± 0.18	5.36 ± 0.07	-0.0081[b]	28.83
BE_1	664.48 ± 0.18	5.37 ± 0.07	-0.0107[b]	28.83
BE_2	663.44 ± 0.31	6.37 ± 0.28	-0.35 ± 0.10	28.83
KE	663.37 ± 0.33	6.49 ± 0.33	-0.43 ± 0.14	28.83
ME_1	662.24 ± 0.23	5.19 ± 0.10	0.00 ± 0.00	34.77
ME_2	662.10 ± 0.61	5.35 ± 0.60	-0.057 ± 0.21	34.77
GGKE	662.23 ± 0.23	5.21 ± 0.10	-0.008[b]	34.77
BE_1	662.23 ± 0.23	5.22 ± 0.10	-0.010[b]	34.77
BE_2	662.12 ± 0.61	5.33 ± 0.61	-0.052 ± 0.22	34.77
KE	662.11 ± 0.62	5.35 ± 0.63	-0.058 ± 0.24	34.77
ME_1	659.97 ± 0.28	5.11 ± 0.11	0.00 ± 0.00	40.91
ME_2	659.70 ± 0.75	5.38 ± 0.69	-0.088 ± 0.23	40.91
GGKE	659.95 ± 0.28	5.13 ± 0.11	-0.0078[b]	40.91
BE_1	659.95 ± 0.29	5.14 ± 0.11	-0.0095[b]	40.91
BE_2	659.71 ± 0.75	5.37 ± 0.70	-0.092 ± 0.24	40.91
KE	659.70 ± 0.77	5.39 ± 0.74	-0.099 ± 0.27	40.91

[a] The authors do not consider this quantity to be physically significant as the pressure measurements are not sufficiently accurate.

[b] Obtained from B_0 and B'_0.

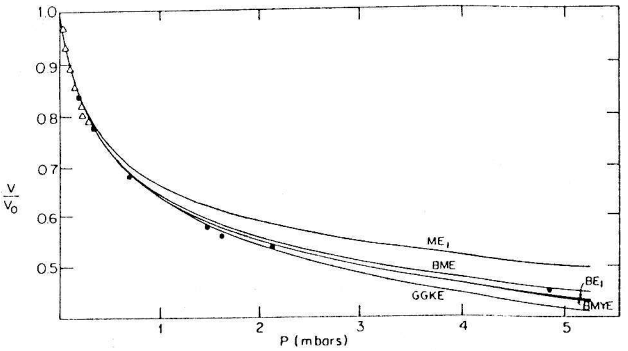

FIG. 2. Extrapolation of pressure-vs-volume data for LiF. The △, ■, and ● are data from Refs. 26, 27, and 28, respectively.

the experimental precision in measuring V/V_0 is 1×10^{-7} and is at least two orders of magnitude better than previous techniques,[24,25] it is still not sufficient by itself to extract reliable information on B''_0 because of the error in measuring pressure. Changing the length measurement data randomly by a few parts in 10^7, has the effect of not only changing the magnitude of B''_0 by an order of magnitude but also results in changing its sign sometimes. Moreover, B''_0 is highly dependent on the functional form of the variation of p with the change in resistance per unit resistance $(\Delta R/R_0)$ of the manganin gauge. If we assume that $p = C(\Delta R/R_0) + D(\Delta R/R_0)^3$ then, as indicated in Table VI, the values that one obtains for B''_0 is considerably different from those given in Table II. [The values listed in Table II are based on the assumption that $p = A(\Delta R/R_0) + B(\Delta R/R_0)^2$. The coefficients (C, D) or (A, B) are determined by knowing $(\Delta R/R_0)$ at the freezing point of mercury at 0 °C and by knowing ΔP_M, the nonlinear parameter.[22]] The B''_0 listed in Table VI are generally smaller in magnitude and hence appear to be in closer agreement with what one obtains from lattice models. Even though the lattice models themselves are not free from any criticism, this would immediately prompt one to speculate on the "exact" functional form for the variation of p with $\Delta R/R_0$ for the manganin gauge. However, one would have to know p to better than one part in a million to be able to conclusively determine the variation of p with $\Delta R/R_0$.

Although the validity of the extrapolation of the pressure-volume data into a high-pressure range is questionable, the extrapolation is made in order to see the discrepancies between the equations of state. Indeed when all the two-parameter equations of state are extrapolated, they are hardly distinguishable up to pressures as high as 100 kbar. As shown in Fig. 2, ME_1 begins to deviate from other equations of state at about 100 kbar, and the discrepancy at 300 kbar between ME_1 and others is approximately 4%. At 700 kbar the deviation increases to about 14%, whereas the discrepancy among the other equations themselves at 700 kbar is only 3%. The Born-Mayer two-parameter static equation of state and BE_1 are virtually indistinguishable in the over-all pressure range up to (~5 Mbar). These equations of state predict V/V_0 in good agreement with the Pagannone Drickamer[26] static compression data and Christian's shock-wave data,[27] both measured below 300 kbar. If one does not question the uncertainties in pressure that arise in the conversion from the shock Hugoniot to pure isothermal conditions, then it would seem that the GGKE gives the best fit if we ignore the data point at 4.8 Mbar.[28]

From the present work we find it impossibel to discriminate between these equations of state. The maximum applied pressure, about 7 kbar, is too small and is not precise enough for the meaningful determination of B''_0 and discrimination between these equations of state for a LiF single crystal having a bulk modulus of about 665 kbar at ambient pressure. For the improvement of equation-of-state data it is at first desirable to simultaneously measure both $V(P)$ by the present apparatus and $B^S(P)$ by ultrasonic technique for the same specimen and second to extend the applied pressure range significantly. It would also require an accurate calibration of the pressure gauge as B'_0 is sensitive to the nonlinear parameter in determining the pressure by the manganin gauge,[22] and B''_0 is significantly dependent on the functional form for the variations of p with $\Delta R/R_0$ for the manganin gauge. In fact, if the pressure P could be measured to the same accuracy as V/V_0 (better than one part in 10^6) the present length measurement system would produce an accurate value of the second derivative of the bulk modulus B''_0, without resorting to ultrasonic measurements.

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