LATTICE MODEL CALCULATION OF ELASTIC AND THERMODYNAMIC PROPERTIES AT HIGH PRESSURE AND TEMPERATURE*

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The elastic constants and the entire frequency spectrum have been calculated up to high pressure for the alkali halides in the NaCl lattice, based on an assumed functional form of the interatomic potential. The quasiharmonic approximation is used to calculate the vibrational contribution to the pressure and the elastic constants at arbitrary temperature. By explicitly accounting for the effect of thermal and zero point motion, the adjustable parameters in the potential are determined to a high degree of accuracy from the elastic constants and their pressure derivatives measured at zero pressure. The calculated Grüneisen parameter, the elastic constants and their pressure derivatives are in good agreement with experimental results up to about 600 K. The model predicts that for some alkali halides the Grüneisen parameter may decrease monotonically with pressure, while for others it may increase with pressure, after an initial decrease.

In addition to giving good estimates of properties at high pressure and temperature, these calculations permit the estimation of the probable errors which arise from using less detailed theories. For pressures up to 0.5 K_0, which correspond to the lower mantle of the Earth and the deep interiors of the other terrestrial planets, simple linear extrapolation of the elastic constants with pressure leads to an error of less than 2% in the density and up to about 5% in the seismic velocities.

1. Introduction

The theoretical treatment of many important geophysical problems often requires that data measured in the laboratory at low pressures be extrapolated to the extreme conditions of planetary interiors. The extrapolation of elastic constants to high pressure is of central importance to the interpretation of seismic velocities. The determination of the adiabatic temperature gradient in the earth depends strongly on the behavior of the Grüneisen parameter under pressure. Uncertainty about the pressure variation of the Grüneisen parameter is still a major problem in the interpretation of shockwave experiments. Although there are many empirical formulas for extrapolating elastic constants or the Grüneisen parameter to high pressure, only two basic approaches to the problem have a firm theoretical basis – finite strain theory and lattice theory.

THOMSEN (1970, 1971, 1972) has extended the fourth-order Lagrangian finite strain theory to treat the elastic properties at arbitrary pressure and temperature. The complete application of this theory requires knowledge of a great many experimental parameters (19 for cubic crystals) and has thus so far been limited to a few simple compounds. However, treatment of the equation of state requires only nine experimental values for input, and the calculation has been carried out recently for 17 cubic compounds (AHRENS and THOMSEN, 1972).

While finite strain theory is based on lattice dynamics, it makes no assumptions about the nature of the interatomic forces. For crystals such as the alkali halides for which the interatomic forces are fairly well understood, the number of input parameters can be greatly reduced by assuming the interatomic forces to be of a particular form. Lattice dynamical models have often been successful in predicting many properties of crystals, using relatively little experimental data as input. Unfortunately, the interatomic forces in complex geological materials are not well understood, and at least for the time being, lattice dynamical extrapolations to high pressure are probably not very accurate for most materials of geological interest. My present calculations are therefore limited to alkali halides having the NaCl structure.

2. Lattice dynamical calculations

2.1. *Background*

Conventional lattice dynamics generally treats the entire frequency spectrum of harmonic vibrations of a lattice at a particular volume. (For a recent review article, see COCHRAN, 1971.) By considering a small perturbation of the volume, many authors (for example, BARRON, 1957; ACHAR and BARSCH, 1971 a,b; NAMJOSHI *et al.*, 1971) have calculated the zero pressure Grüneisen parameter as a function of temperature, getting fairly good agreement with experiment. By assuming a functional form of the interatomic potential, a number of authors have attempted to predict the elastic properties and equation of state of the NaCl lattice at high pressure (ANDERSON and LIEBERMANN, 1970; SAMMIS, 1970, 1971; ANDERSON, 1970; ANDERSON and DEMAREST, 1971; BARSCH and SHULL, 1971; DEMAREST, 1972). None of these authors attempted to treat the entire frequency spectrum at high pressure, although ANDERSON and DEMAREST (1971) did calculate a Grüneisen parameter based only on the low-frequency acoustic modes of vibration. In the present paper, I have extended previous work (DEMAREST, 1972) to include the entire frequency spectrum. The quasiharmonic approximation, in which the frequencies are assumed to be functions of volume but not of temperature, is used. The results are a set of equations which can be used to predict virtually any thermodynamic property of the crystal at arbitrary pressure and temperature.

2.2. *Central force model*

I have assumed that the potential energy per ion pair of the crystal is given by

$$\tilde{\phi} = \sum_{i=1}^{\infty} \pm \frac{z^2 e^2}{r_i} + \sum_{i=1}^{6} b \exp\left(-r_i/\rho\right)$$
$$+ \frac{1}{2} \sum_{i=1}^{12} \varepsilon_0 \left[\left(\frac{r_m}{r_i}\right)^{12} - 2\left(\frac{r_m}{r_i}\right)^{6}\right]. \quad (1)$$

The tilde over ϕ indicates that vibrational effects are neglected.

The first term is the electrostatic energy summed over all ions in the lattice. The second term gives the repulsive energy between nearest neighbours, and the third term gives the interaction between anions.

There is little justification for using the Lennard–Jones 6–12 potential between anions, although its qualitative features were verified by WEIDNER and SIMMONS (1972) and by DEMAREST (1972). The neglect of noncentral or multibody forces in this model will not cause serious error in the alkali halides, where such effects can be shown to be small, but the central force assumption is invalid for MgO, AgCl and AgBr, and may be equally invalid for many geophysically important materials.

A more serious defect of the model is the neglect of the polarizability of the anion. Although polarizability does not affect the elastic constants in a centrosymmetric lattice, it has a strong effect on the optic modes of vibration. Treatment of the polarizability is possible through the shell model. Its neglect in the present rigid ion model calculation leads to calculated optic frequencies which are 10% to 40% too high at zero pressure. This in turn will lead to an underestimation of the specific heat and will directly affect the accuracy of the calculated mode Grüneisen parameters, which are discussed in the next section. Since the macroscopic Grüneisen parameter represents an average over all modes of vibration, the error caused by this neglect of polarizability will probably cancel to some extent in the summations. The resulting error in the Grüneisen constant should not be more than about 10%.

The equations for the pressure, the elastic constants and their pressure derivatives in the model were derived in DEMAREST (1972). The procedure for calculating the frequency of vibration for arbitrary wavevector, based on a potential function such as the above, has been adequately discussed in COCHRAN's (1971) review article. Detailed applications to the NaCl lattice are given by KELLERMANN (1940), COWLEY (1962) and PECKHAM (1967). The mode Grüneisen parameters, $\gamma_i = \partial \ln \nu_i / \partial \ln V$, can be calculated by the straightforward application of perturbation theory (WALLACE, 1972, p. 179).

2.3. *Thermal effects*

The total energy in the lattice is the sum of two terms, corresponding to the static lattice and the vibrational energy:

$$\phi = \tilde{\phi} + \sum_i h\nu_i \left[\frac{1}{2} + (\exp\left(h\nu_i/kT\right) - 1)^{-1}\right]. \quad (2)$$

In this equation the ν_i are the frequencies of vibration of the normal modes. In my calculations, I have carried

out the summation over a representative sample of 282 frequencies corresponding to 47 wavevectors. WALLACE (1972) has discussed the procedure for carrying out the summation.

The vibrational contribution to pressure is obtained by differentiating eq. (2):

$$P = \tilde{P} + V^{-1} \gamma_e E_{vib},$$ (3)

$$\gamma_e \equiv \sum_i \gamma_i E_i / (\sum_i E_i).$$ (4)

E_{vib} is the vibrational energy corresponding to the summation term in eq. (2), and E_i is the ith vibrational term within the summation. V is the volume. The vibrational pressure term in eq. (3) includes the effect of zero point motion. In this respect it differs from the expression of BARRON (1955), who chose to incorporate the zero point effect into his potential $\tilde{\phi}$.

Except at high temperature, γ_e is not the same as the thermal Grüneisen parameter γ_{th}, which is given by

$$\gamma_{th} \equiv \frac{V \beta K_T}{C_v} = \frac{\sum \gamma_i C_{vi}}{\sum C_{vi}},$$ (5)

where β is the volume thermal expansion coefficient, K_T is the isothermal bulk modulus, C_v is the heat capacity at constant volume, and C_{vi} is the contribution of an individual mode to the heat capacity.

Although it is possible to develop an analytic expression for the thermal corrections to the isothermal bulk modulus K_T (WALLACE, 1972, p. 194). I have determined this correction by numerical differentitation. The formula for converting K_T to the adiabatic bulk modulus K_s is well known. The thermal correction to dK_s/dP was also determined by numerical differentiation.

The quasiharmonic approximation suggests that there should be no thermal correction to the shear elastic constants. However, at least for the alkali halides, this assumption is empirically more correct for the thermodynamic than the effective elastic constants, and I have made thermal corrections accordingly. [The effective elastic constants are those which appear in the equations of motion. The effective shear constants are less than the thermodynamic ones by the quantity P. For further discussion of this distinction, see THURSTON (1965).]

2.4. Determination of arbitrary parameters

There are five arbitrary parameters in eq. (1): z, b, ρ, ε_0 and r_m. These were determined in order to make the calculated and experimental values of five quantities agree: $P = 0$ (the equilibrium condition), K_s, dK_s/dP, the shear elastic constant C_{44} and its pressure derivative dC_{44}/dP. The elastic constants and their pressure derivatives can be measured very accurately by modern acoustical experiments and are a very sensitive measure of the interatomic forces.

It is important to point out several differences between the above procedure and those used by others. The vibrational corrections to the pressure, elastic constants and pressure derivatives, discussed in the previous section, permit a calculation of thermal effects which is exact within the framework of the quasiharmonic approximation. Without this exact thermal treatment, it has been necessary to extrapolate the experimental values to either zero temperature (DEMAREST, 1972) or to a static reference state (SAMMIS, 1971), necessitating experimental data at several temperatures.

There are several alternatives to fitting the arbitrary parameters to the pressure derivatives of the elastic constants. For example, in a similar model, SAMMIS (1971) assumed that the parameters in the Lennard–Jones 6–12 potential between anions were the same as for the isoelectronic inert gases. In their model for the NaCl structure, BARSCH and SHULL (1971) and CHANG and BARSCH (1971) used parameters estimated by TOSI (1964) and others. This procedure sometimes leads to rather poor agreement with experimental elastic constants and pressure derivatives and is therefore inappropriate for extrapolations to high pressure.

In calculations similar to the present ones (DEMAREST, 1972), I tried to correct for thermal effects by extrapolating the elastic constants to zero temperature. The parameters in eq. (1) which fitted the elastic constant data for 12 alkali halides were all reasonable, although the anion–anion force constant ε_0 was 5–10 times larger than SAMMIS (1971) had assumed.

With the more exact thermal treatment of the present paper, the parameters are slightly different. The improvement in the effective ionicity Z is noteworthy. In the earlier calculations the ionicity varied from 0.86–1.03, in a manner which could not be explained physically. When the explicit thermal corrections are included, the variation is from 0.96–1.04. Most of the remaining variation can be explained by errors in the measured elastic constants. I regard this relatively small variation

of Z among 12 compounds to be dramatic proof that eq. (1) is a good approximation to the interatomic forces in alkali halide crystals.

3. Comparison with experiment

Because explicit thermal corrections are made in these calculations, it is possible to compare theory to experiment over a wide range of temperatures. Of perhaps greatest interest is the Grüneisen parameter discussed in subsection 2.2. The Grüneisen parameter calculated from the normal mode spectrum of NaCl by eq. (5), γ_{th}, is compared with experimental results over a wide temperature range in fig. 1. γ_e, which occurs in
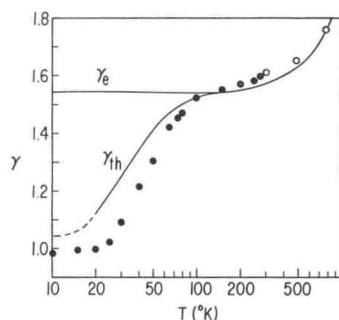
Fig. 1. Grüneisen parameter of NaCl versus temperature in NaCl. ● – WHITE (1965); ○ – SPETZLER et al. (1972); — – theoretical calculation.

the equation of state (eq. 3) is also shown. The 10% agreement with experiment approaches the accuracy of others, who have used much more detailed models than the present one, and whose calculations have been limited to zero pressure (for example, ACHAR and BARSCH, 1971a, b; NAMJOSHI et al., 1971).

My theoretical calculation of the adiabatic and iso-thermal bulk moduli are compared with experimental data over a wide range of temperatures, in fig. 2. The agreement is excellent up to about 600 K. The calculated shear elastic constant C_{44} (not shown) is within 1 or 2% of experimental values up to at least 800 K.

The other shear elastic constant, $C_s \equiv \frac{1}{2}(C_{11} - C_{12})$, is the only elastic constant which is not used as an input parameter. Its value is determined essentially by the Cauchy relation, $\tilde{C}_{12} - \tilde{C}_{44} = 2\tilde{P}$, which is a result of the assumption of a potential based on two-body interactions. In NaCl, the calculated value of C_s differs from experiment by about 7%, while the pressure derivative is in error by 15%.
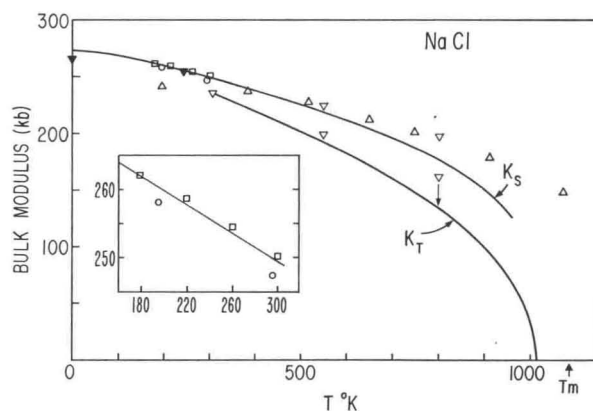

Fig. 2. Adiabatic and isothermal bulk moduli of NaCl versus temperature. □ – GHAFELEHBASHI et al. (1971); ○ – BARTELS and SCHUELE (1965); ▽ – SPETZLER et al. (1972); ▼ – LEWIS et al. (1962); △ – SLAGLE and McKINSTRY (1967); — – theoretical calculation.

A comparison of the predicted pressure derivatives of K_s and C_{44} is given in fig. 3, over a wide temperature range. The agreement of dC_{44}/dP is fairly good over the entire temperature range. The predicted dK/dP rises above the experimental data at about 400 K, with the disagreement becoming serious above about 600 K. The unusually low value of dK/dP reported by GHAFELEHBASHI and KOLIWAD (1970) at 180 K is inconsistent with the earlier result of BARTELS and SCHUELE (1965) at 195 K, and is hard to explain in terms of the quasiharmonic approximation.

It is apparent that more sophisticated thermal corrections than the quasiharmonic approximation will be necessary above about 600 K. The explicit in-clusion of fourth-order vibrational effects begins to differ from the quasiharmonic approximation at about 300 K. Its inclusion in the present model calculations
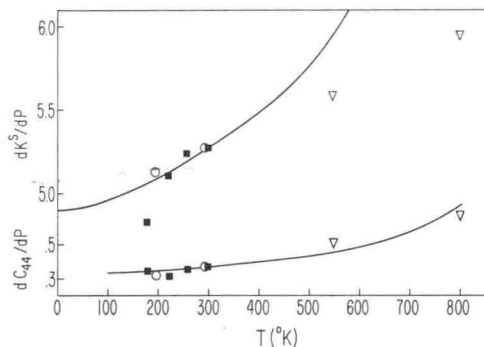

Fig. 3. Pressure derivative of K_s and C_{44} versus temperature in NaCl. Symbols as in fig. 2.

would be straightforward (COWLEY, 1971; GLYDE and KLEIN, 1971).

The second pressure derivatives of the elastic constants have been reported for NaCl by SPETZLER *et al.* (1972), and for five other alkali halides by CHANG and BARSCH (1971) and BARSCH and SHULL (1971). Predictions of my model are in fair agreement with the results of Barsch and his coworkers; however, neither my model nor that of SAMMIS (1971) can explain the unusually large values reported for NaCl. The measurement of the second pressure derivatives is a difficult task, and while this disagreement is cause for concern, a full evaluation cannot be made until the experimental results on a single compound are agreed upon by more than one laboratory.

4. Extrapolation to high pressure

4.1. *The elastic constants*

The procedures discussed in the preceding two sections permit the calculation of the elastic constants to high pressure at arbitrary temperature. The shear elastic constant C_{44} in NaCl is of particular interest for two reasons. First, a relatively low value of C_{44} at high pressure may be associated with the phase transition to the CsCl structure discovered by BASSETT *et al.* (1968) at 300 kbar. Second, a number of theorists have speculated about the variation of C_{44} with pressure, and it is useful to compare their predictions to this theory. A comparison of several theoretical extrapolations of C_{44} versus pressure is given in fig. 4. SAMMIS's (1971) lower curve results from a potential similar to this paper, but neglecting the anion–anion interaction. This results in a value of C_{44} which decreases much too rapidly with
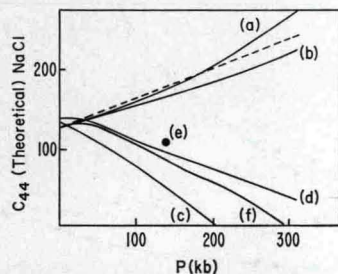

Fig. 4. Comparison of different theoretical extrapolations of shear constant C_{44} in NaCl to high pressure. (a) this paper; (b) DEMAREST (1972); (c) SAMMIS (1971), no anion interaction; (d) SAMMIS (1971), anion interaction; (e) WEIDNER and SIMMONS (1972); (f) THOMSEN (1972); - - - – linear extrapolation.

pressure and reaches zero before the observed phase transition. Similar results were achieved by ANDERSON and DEMAREST (1971) using a similar model. By including an anion interaction of the same strength as measured between inert gas ions, he obtained the higher curve, which still does not fit the experimental pressure derivative at zero pressure. A much stronger anion–anion force is needed to explain the pressure derivative of C_{44}. WEIDNER and SIMMONS (1972) predict C_{44} at only one pressure, assuming that the anion and coulombic forces are the same as in LiCl at the same volume. THOMSEN (1972) used finite strain theory to predict C_{44} at high pressure, using a model prediction of d^2C_{44}/dP^2 as an input parameter, and predicting that C_{44} will vanish right at the observed transition.

My own predictions differ markedly from the others. My predicted curve for C_{44} is at first slightly concave downward, then upward, and stays close to the linear extrapolation (dashed line). The change in sign of d^2C_{44}/dP^2 which may be an explanation for the disagreement with the finite strain theory result, which does not permit such a possibility.

There is unfortunately little experimental data to determine which of the curves in fig. 4 is most nearly correct. However, we may ask whether or not it is reasonable for C_{44} to become as weak as is predicted by SAMMIS (1971) or THOMSEN (1972). My calculations on eight alkali halides in which phase transitions to the CsCl structure are well known showed that the predicted value of C_{44}/K at the transition was about the same for all eight compounds (DEMAREST, 1972). The present calculations suggest that the value is 0.185 ± 0.035. This result cannot be disputed in RbCl, RbBr and RbI, which undergo transitions at pressures within the range of acoustical experiments, and cannot be seriously in error for the potassium halides which undergo transitions at a low enough pressure that linear extrapolation of the elastic constants is still fairly accurate. I believe that it is unlikely that NaCl is so different from the other alkali halides that C_{44}/K will decrease to 0 as predicted by THOMSEN or to 0.03 as predicted by SAMMIS. I therefore believe that my own prediction that $C_{44}/K = 0.17$ at the transition is the most accurate.

4.2. *The Grüneisen parameter*

Assumptions of how the Grüneisen parameter γ

varies with volume are important to the reduction of shock wave data, to the determination of the adiabatic temperature gradient in the Earth, and to the more general problem of the equation of state of solids, which was discussed in subsection 2.2. The uncertainty in the variation of γ with volume has been discussed recently by ANDERSON (1968) and by KNOPOFF and SHAPIRO (1969).
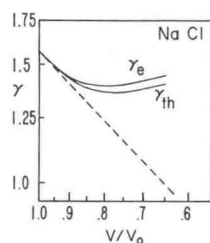

Fig. 5.   Model calculation of Grüneisen parameter in NaCl as a function of volume. — – lattice theory (this paper); - - - – finite strain theory (AHRENS and THOMSEN, 1972).
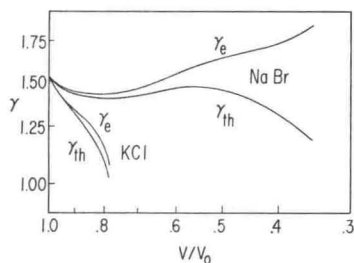

Fig. 6.   Grüneisen parameter in NaBr and KCl calculated from lattice theory as a function of volume.

The predicted variation of γ with volume at 300 K is given in fig. 5 for NaCl and in fig. 6 for NaBr and KCl. Initially, γ decreases with compression, in accord with many simple theories. In KCl, the behavior is nearly linear up to the phase transition. In NaCl, NaBr and the other sodium halides, the model calculation for γ reaches a minimum and then increases with compression. This is consistent with ANDERSON's (1968) prediction that the behavior of $\gamma(V)$ would be different at high pressure than at low pressure.

The present prediction of $\gamma\ (V)$ and the prediction of finite strain theory begin to diverge at about $V/V_o = 0.8$, which is the limit of accuracy claimed for finite strain theory by AHRENS and THOMSEN (1972).

In earlier lattice model calculations, based only on the low-frequency acoustic modes, ANDERSON and DEMAREST (1971) showed that γ might sharply decrease shortly before the occurrence of a phase change which resulted from the softening of certain vibrational modes. There is some indication of this effect for KCl in fig. 6, but my present calculation indicates that this effect is negligible in the 12 alkali halides which I have studied because the phase change invariably takes place before any of the modes become very weak, for example, when $C_{44}/K = 0.18$ instead of 0.

Because γ depends on the volume derivative of the frequencies, its accuracy is uncertain, but probably less than the accuracy of the elastic constants. A different assumed form of the interatomic potential might lead to different results. Since the same set of assumptions was used to calculate $\gamma(V)$ in KCl and NaBr, the conclusion that $\gamma(V)$ can have sharply dissimilar behavior for different compounds of the same crystal structure is probably valid, as is the conclusion that for some compounds the Grüneisen parameter may increase with pressure, after an initial decrease.

5. Accuracy of high-pressure extrapolations

Data on the elastic constants and their first pressure and temperature derivatives are available for a number of geologically important materials (for example, ANDERSON et al., 1968; KUMAZAWA and ANDERSON, 1969). Although geological materials have been treated within the framework of lattice dynamics (for example, SAMMIS, 1970, 1971; WEIDNER and SIMMONS, 1972; STRIEFLER and BARSCH, 1972), these calculations are not well suited to extrapolation to high pressure because they do not agree with the experimental pressure derivatives in some cases, or in other cases do not assume a functional form for the interatomic potential, and thus cannot be extrapolated to high pressure. Accurate versions of finite strain theory (THOMSEN, 1972) are presently inapplicable to most geological materials because the required second pressure derivative data are lacking. Geophysicists are therefore often forced to make use of relatively naive extrapolation formulas with little knowledge of what sort of accuracy can be expected.

I have attempted to make rather crude estimates of the type of errors to be expected from using simple approximations to the equation of state and for the determination of the elastic wave velocities at high pressure, by seeing at what pressures different theories begin to diverge. The density and elastic wave velocities have been calculated based on a linear extrapolation

of the elastic constants (as in the Murnaghan equation of state) and compared to the lattice theory calculations described in his paper and other calculations based on a nearest-neighbor repulsive force of the form b/r^n rather than be^{-r}/p. The first pressure derivatives of the elastic constants are assumed to be known.

The results of these comparisons are given schematically in figs. 7 and 8. Fig. 7 compares the density cal-
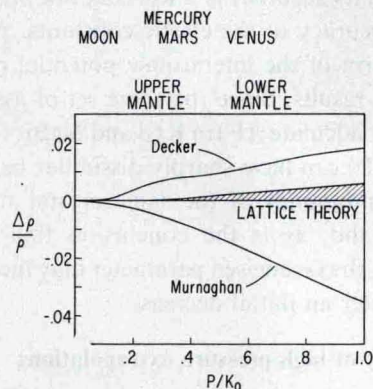

Fig. 7. Deviation of different equations of state calculations in NaCl from this paper, as a function of reduced pressure. For geological materials, the terrestrial planets or regions of the Earth corresponding to particular reduced pressures are represented by captions along the top axis.

culated from different equations of state for NaCl; fig. 8 compares the typical deviation of the calculated velocities from the present calculation for a linear extrapolation of the elastic constants, and for minor changes in the repulsive force, which represents for the present the inherent uncertainty of lattice theory.

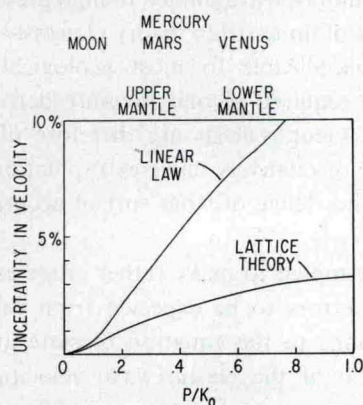If we assume a certain similarity between the high-

Fig. 8. Uncertainty in the estimated velocities in alkali halides as a function of reduced pressure. The captions on the top axis have the same meaning as in fig. 7.

pressure behavior of alkali halides and geological materials, we can estimate the accuracy of the application of simple formulas to problems of planetary interiors. Toward this end, captions above figs. 7 and 8 designate the regions of the Earth or deep interiors of the terrestrial planets which correspond to particular values of the reduced pressure for typical geological materials such as olivine or MgO.

This assumption implies that the density of geological materials under upper mantle conditions can probably be estimated to an accuracy of 1% and to an accuracy of 2% in the lower mantle.

There is a good chance that the sound velocities in olivine at a depth of 400 km ($P/K_0 = 0.1$) can be estimated to an accuracy of about 1%, but at greater depths the accuracy of any extrapolation will be much worse. Even the uncertainty of lattice theory lies well above the uncertainty in seismic velocities ($\approx 1\%$) through most of the Earth's interior. The full interpretation of presently available seismic data awaits significant improvement of theoretical methods of estimating elastic properties of geological materials at high pressure.

6. Conclusions

A very simple assumption about the nature of the interatomic potential in alkali halides, with only five arbitrary parameters, permits the calculation of the elastic constants and Grüneisen parameter at arbitrary pressure and temperature. The calculations are in excellent agreement with experiments at low pressure up to about half the melting temperature. The use of the pressure derivatives of the elastic constants in fitting the arbitrary model parameters is important if accuracy is to be obtained at high pressure.

The determination of a good interatomic potential for oxides and silicates would permit the application of this type of calculation to geologically important materials. Although this difficult problem has not yet been solved, several results of the application of the theory to alkali halides are of general interest.

Simple assumptions on the volume variation of the Grüneisen parameter may often be in serious error at volume compressions of greater than about 15%. The qualitative features of $\gamma(V)$ can vary, even among similar compounds, and may increase with pressure in some instances after an initial decrease.

Although simple equations of state will give accurate values of the density at fairly high pressure, simple estimates of the elastic properties and seismic wave velocities are probably not very accurate in most regions of geological importance.

Acknowledgment

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