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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.

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