# APPLICATION OF HYDROSTATIC PRESSURE AND SHOCK WAVE DATA TO THE THEORY OF COHESION IN METALS

E. S. FISHER,* M. H. MANGHNANI, AND K. W. KATAHARA

*Hawaii Institute of Geophysics, University of Hawaii*
*Honolulu, Hawaii 96822, U.S.A.*

The parameter $K' = dK/dP$ (where K is isothermal or adiabatic bulk modulus) is useful in analyzing interatomic forces or interactions. A model is presented that is useful in predicting $K'$ values in certain close-packed and other metallic structures. K is assumed to consist of two additive components: $K_F$, the free-electron Fermi gas component, and $K_{SR}$, the interatomic short-range repulsive component derived from a Born-Mayer approximation. At infinitely large molar volumes, only $K_F$ is important and $K'$ should approach a value of 5/3. With decreasing molar volume, the $K_{SR}$ contribution of $K'$ increases through the relation: $K'_{SR} = K_{SR}(B+1)/3K_T$, where $K_T$ is isothermal bulk modulus, B is the "hardness" parameter in the Born-Mayer expression for the energy of interatomic repulsion, and the ratio $K_{SR}/K_T$ is assumed to vary with $1/\Omega_o$ where $\Omega_o$ is the initial molar volume. The $K'$ values from the ultrasonic and shock wave data for metals have been selectively used to compare with the above model. It is shown that the data for the close-packed metal structures, h.c.p. and f.c.c., are reasonably consistent with the model, whereas the limited data for b.c.c. transition metals indicate that $K'$ for this group is influenced by electron band structure and other contributions to the elastic moduli.

## Introduction

An analysis of the data for the pressure derivatives of bulk modulus, $K' = dK/dP = (\partial K/\partial P)_T$ as $P \to 0$ (K denotes both isothermal and adiabatic modulus), shows that for purely ionic solids the ultrasonic value of this parameter seldom varies from its range of 4 to 6, and that for a given structure the parameter value shows no systematic relationship to unit cell volume (for example, in alkali halides). In oxides and simple silicates, which are partly ionic and partly covalent, $K'$ tends to increase with decreasing density at constant mean atomic weight [1].

The conclusions reached from a Born model treatment of the data for ionic compounds of NaCl-structure type (which include some oxides) are that the variations of dK/dP are primarily a function of the repulsive parameter, n, which is derived from a $1/r^n$ type of interatomic repulsive potential [2] and which is numerically related to the repulsive parameter, B, in the Born-Mayer form of the potential for ion-core interactions.

In contrast to ionic solids, metals show a wider variation in values of dK/dP, ranging approximately from 3 to 7. In addition, the reported dK/dP values for metals appear to increase continuously with decreasing molar volume (see Figure 1). The purpose of this paper is to show that most of the data are indeed consistent with a model for the bulk modulus which contains two components: a free electron Fermi gas component, and a Born-Mayer interatomic repulsive component. This simple treatment shows that the two-component model is a reasonably good physical model for the cohesive forces in f.c.c. and h.c.p. metals, but may not

be valid for the b.c.c. transition metals where the electron band structure energy makes an important contribution to the elastic moduli.

## Data

The values of $K'_T = dK_T/dP$ that we have used in this study and which are plotted in Figure 1 were obtained from direct ultrasonic measurements that appear in the literature [3-13] or from recent unpublished measurements as noted in Table 1. In this survey we were somewhat selective and did not include all the unpublished values. Excluded are certain f.c.c. metals (for example, Zn, Cd, and Pb) with very high $K'$ values. These metals have high compressibility, and it is regarded that anomalous properties and experimental errors may have contributed to atypical $K'$ values.

In addition to the ultrasonic data, we have relied to some extent on $K'_T$ values derived from shock wave data using the second order Birch-Murnaghan equation [13]:

$$P = \frac{3}{2K_{T_0}} (\eta^{7/3} - \eta^{5/3}) \left[1 + \frac{3}{4} (K'_T - 4) \right.$$
$$\left. \cdot (\eta^{2/3} - 1) + \ldots\right] \qquad (1)$$

where $K_{T_0}$ is the initial bulk modulus, P is the hydrostatic pressure, and $\eta = V(0)/V(P)$ is the ratio of initial volume at pressure P. Since $K_{T_0}$ is known,

$$K'_T = 4 + \frac{P - \frac{3}{2} K_{T_0} (\eta^{7/3} - \eta^{5/3})}{\frac{9}{8} K_{T_0} (\eta^{7/3} - \eta^{5/3})} \qquad (2)$$

can be calculated at each $(P, \eta)$ point along the Hugoniot; the $(P, \eta)$ points along the Hugoniot are sufficiently close

*Research affiliate, permanent address, Argonne National Laboratory, Argonne, Illinois 60439 USA.