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# Elastic Constants of the Central Force Model for Three Cubic Structures: Pressure Derivatives and Equations of State[1]

ORSON L. ANDERSON

*Lamont-Doherty Geological Observatory of Columbia University*
*Palisades, New York 10964*

The case of the generalized repulsive potential in the central force approximation is used in Born's lattice theory to derive the elastic constants versus pressure for the NaCl, CsCl, and ZnS structures. The equations are rearranged so that $c_{ij}$ is a function of $K$ and $P$, the bulk modulus and pressure. The isothermal equation of state relates $K$, $P$, and the density $\rho$, so that the elastic constants are specific functions of the relation between $K$ and $P$, and $\rho$ and $P$. As a special case of the theory, the parameter in the repulsive potential $n$ is evaluated by the measured value $K_0'$. The theory shows that the simple repulsion $v(r) = b/r^n$ accounts for the experimental results, except for a small term due to noncentral binding.

## INTRODUCTION

It has been emphasized in several recent publications [*Soga and Anderson,* 1967; *Soga,* 1969; *Anderson,* 1968; *Anderson and Liebermann,* 1970] that the shear velocity decreases with increasing pressure for structures with low coordination. This result has several geophysical applications and is of interest to lattice dynamical theories.

The fact that the shear velocity decreases with pressure is connected to the stability of the structure, because the lattice becomes unstable when a shear constant vanishes [*Born,* 1940; *Misra,* 1940]. Obviously, if a shear constant vanishes at the transition pressure, it must decrease with pressure in a range of pressure just below the transition pressure. The question arises, under what circumstances will an elastic constant, $c_{ij}$, decrease with pressure, $P$.

In this paper I present the equations of the elastic constants as a function of pressure for NaCl, CsCl, and ZnS in the case of a central force model, where the attractive energy is coulombic and the repulsive energy is generalized. This is called the generalized ionic model. Some rather tentative extensions are made to the case of noncentral bonding.

In the derivations I make two drastic assumptions. The first is that the thermal pressure can be ignored; consequently, the results are only strictly applicable at absolute zero. The second is that only first nearest neighbors are considered in the repulsion. These restrictions are slightly relaxed in subsequent sections to show that the assumptions affect only slightly the numerical results of the elastic constants $c_{ij}$ and $dc_{ij}/dp$. After the elastic constants and the pressure derivatives are found for the generalized ionic model, the special case of the repulsion law $b/r^n$ is considered in detail. This law has been used many times before (*Barron* [1957]; *Blackman* [1957, 1958]; *Reddy and Ruoff* [1965]; R. W. Roberts, private communication, 1968), but it is extended to find the generalized isothermal equation of state, and the pressures derivatives of the elastic constants evaluated at zero pressure.

## LATTICE DYNAMIC EQUATIONS FOR DIATOMIC IONIC CRYSTALS

The fundamental theory is due to *Born* [1926] and *Born and Goppert-Meyer* [1933], and the method of defining elastic constants using this theory closely follows that of *Barron* [1957] and of *Blackman* [1957, 1958].

Consider the lattice potential (energy per

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unit cell) for a diatomic lattice where the ion–ion distance is $r$.

$$\phi = A_m(Z_1Z_2e^2/r) + Mv(r) \qquad (1)$$

where $A_m$ is the Madelung constant obtained by summing $(Z_1Z_2e^2)/r$ over all lattice sites, and where $M$ is the coordination number arising from summing the repulsion over next nearest neighbors. The repulsive potential $v(r)$ is unspecified except that it be a function of $r$, and that it vary so rapidly with $r$ that only first neighbors of type $k'$ need be considered around an ion of type $k$.

The pressure is found from (1) by the operation

$$P = -\frac{d\phi}{dV} = -\frac{r}{3V}\frac{d\phi}{dr}$$

$$= -\frac{A_m}{3Vr}Z_1Z_2e^2 - \frac{r}{3V}M\frac{dv}{dr} \qquad (2)$$

Partial derivatives are not used since all equations are understood to be taken under isothermal conditions.

Equilibrium establishes that

$$A_m\frac{Z_1Z_2e^2}{V_0r_0} = -\frac{r_0}{V_0}M\left(\frac{dv}{dr}\right)_0 \qquad (3)$$

Thus

$$P = \frac{A_m}{3V_0r_0}Z_1Z_2e^2 \cdot\left[\left(\frac{r(dv/dr)}{r_0(dv/dr)_0}\right)\left(\frac{\rho}{\rho_0}\right)^{2/3} - \left(\frac{\rho}{\rho_0}\right)^{4/3}\right] \qquad (4)$$

The bulk modulus is given by

$$K = \rho\frac{dP}{d\rho} = \frac{Mr}{9V}\left[r\frac{d^2v}{dr^2} - 2\frac{dv}{dr}\right] - \frac{4}{9}A_m\frac{Z_1Z_2e^2}{rV} \qquad (5)$$

The value of $K$ at $P = 0$, $K_0$, is obtained from (5) and (3)

$$K = \frac{Mr_0^2}{9V_0}\{\nabla^2v(r)\}_0 = \frac{Mr_0^2}{9V_0}\{\nabla^2\phi\} \qquad (6)$$

where $\nabla^2$ is the Laplacian operator

$$\nabla^2 = (d^2/dr^2) + (2/r)(d/dr)$$

Take

$$\frac{K_0}{\alpha} = A_m(Z_1Z_2e^2/V_0r_0) \qquad (7)$$

For one important repulsive function, $v(r) = b/r^n$, $\alpha$ has a simple interpretation. In this case $\{\nabla^2v(r)\}_0 = -(n-1)(dv/dr)_0$.

Using (6) and (3), $\alpha = (n-1)/9$, a number varying between 0.5 and 1.5 but typically unity. We shall assume that for all reasonable potentials $\alpha$ is a number between 0.5 and 1.5 that is a measure of the strength of the repulsive potential. The variation of $\alpha$ with pressure depends upon the pressure variation of the valence product $Z_1Z_2$, if any.

The bulk modulus, (5), can also be written as

$$K = K^R + K^e = \frac{M}{9}\frac{r}{V}\left[r\frac{d^2v}{dr^2} - 2\frac{dv}{dr}\right] - \frac{4}{9}\frac{K_0}{\alpha}\left(\frac{\rho}{\rho_0}\right)^{4/3} \qquad (8)$$

where the first term is the repulsive contribution to $K$, and where the second term is the Coulombic contribution to $K$.

The equations for the elastic constants equivalent to (8) are now considered. We have, in Born's notation,

$$(c_{\alpha\beta,\gamma\lambda}) = (c_{\alpha\beta,\gamma\lambda})^e + (c_{\alpha\beta,\gamma\lambda})^R$$

and

$$C = C^e + C^R$$

$$D = D^e + D^R$$

where $C$ and $D$ are the constants required for a noncentrosymmetric lattice in which the calculated value of $c_{44}$ for the centrosymmetric lattice is modified by subtracting $C^2/D$. The appropriate lattice sums are well known [*Cowley*, 1962]. We shall use them in the form given in Tables 1 and 4 of the paper by *Anderson and Liebermann* [1970]. Using these sums, we find the general solutions for elastic constants, which are listed as follows: