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Second Order Elastic Constants of NaCl

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ABSTRACT: The complete set of second order elastic constants of NaCl is obtained using the finite strain elasticity theory by considering interactions up to three nearest neighbors of each molecule in the unit cell. The energy density is then compared with the strain dependent lattice energy density obtained from the continuum model approximation to obtain the expressions for the second order elastic constants of NaCl. The second-order potential parameters are obtained from the measured second-order elastic constant of NaCl.

KEYWORDS: Non linear Properties, elastic constants, NaCl

I. INTRODUCTION

NaCl is an important material and a typical ionic solid used as a pressure gauge in laboratory measurements of compression data. NaCl has a stable structure (B1) up to a pressure of about 30GPa, and its melting temperature is nearly 1074 K.

The elastic property of materials is of much importance in many areas of physics and chemistry [1]. Elastic properties are important because they relate to various fundamental solid-state phenomena [2]. By knowing the elastic constants of a material, it is easy to understand the mechanical properties of the materials [3]. The elasticity of a cubic crystal can be specified completely by the three independent second-order elastic constants C_{11} , C_{12} , C_{44} . [4].

II. THEORY

The method of homogenous deformation [5] is used for the determination of the strain energy density of NaCl. The elastic properties are expressed by means of the derivatives of ϕ with respect to atomic displacements when the lattice is deformed. Expressions for the elastic constants are obtained in terms of parameters of the generalized theory[6]. The potential ϕ of the lattice can be expanded in Tayler series as

where l refers to the nearest neighbors. $O'\phi, O''\phi$ are the first, second and third-order co ordinate derivatives of the potential function ϕ .

If the atoms suffer displacement because of the deformation of the lattice, the potential due to two-body interactions arising from three nearest neighbors can written as

$$\varphi' = \varphi + \frac{1}{2} \sum_{N=1}^{3} \sum_{\mu=1}^{4} \left\{ \frac{1}{2} k_2 \left[R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} \cdot R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} - R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} \cdot R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} \right]^2 + \frac{1}{6} k_3 \left[R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} \cdot R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} - R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} - R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} - R \begin{pmatrix} L & L+N \\ \mu & \mu' \end{pmatrix} \right]^3 \right\}$$
(2)



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where k_2 and k_3 are second - and third - order potential parameters respectively. On comparing with the strain dependant lattice energy density expression from the continuum model approximation,

$$U = \frac{1}{2} \sum_{ijkl} C_{ijkl} \eta_{ij} \eta_{kl} + \frac{1}{6} \sum_{ijklmn} C_{ij,kl,mn} \eta_{ij} \eta_{kl} \eta_{mn} + \dots \dots$$
(3)

Equating coefficients of similar terms in $\eta_{ii} \eta_{kl}$, we get the expression for the second order elastic constants as

$$C_{11} = 46.79 k_2'$$

$$C_{12} = 12 k_2'$$

$$C_{44} = 12 k_2'$$
(4)
where $k_2' = \frac{k_2 a^4}{V_z}$ and V_z is the volume of unit cell of NaCl.

The potential parameter k_2 has been obtained by substituting the value of $C_{11} = 48.74$ Gpa in equation (4). The values of second order elastic constants for NaCl are obtained from equation (4) and are given in table [I] along with reported values. Here we have chosen C_{11} calculated by U. Ray [7] to determine the potential parameter k_2 and its value thus

obtained is
$$\begin{pmatrix} a^4 \\ V_Z \end{pmatrix} k_2 = 0.1765$$
 GPa.

Table 1. Second-order elastic constants of NaCl (In GPa) along with the measured values

Reference	C ₁₁	C ₁₂	C ₄₄
Present work	48.74	12.5	12.5
U. Ray [7]	48.74	12.4	12.6

III. EXPERIMENTAL RESULTS

The second order elastic constants [SOECs] of NaCl are given in Table1. C_{11} and C_{12} are 48.74 Gpa and 12.5 Gpa respectively, while the corresponding values of C_{11} and C_{12} obtained by U. Ray [7] are 48.74 Gpa and 12.4 Gpa respectively. While C_{44} is 12.5 Gpa and the corresponding value of C_{44} obtained by U. Ray is 12.6 Gpa.

IV. CONCLUSION

The anisotropy factor A, defined as $A = 2C_{44}/(C_{11}-C_{12})$, is calculated for most materials is smaller than 1. The present value of the anisotropy factor is 0.69. U. Ray [7] obtained the value for A as 0.69. The Bulk modulus is defined as $B = (C_{11}+2C_{12})/3$. U. Ray [7] calculated the Bulk modulus of NaCl as 24.64. Whereas the present value for the Bulk modulus is 24.58.

Martins [8] criteria have been used for testing the numerical validity of SOECs of cubic compounds. According to Martin, the elastic constants should satisfy the relation

 $A = (7/6) 2 C_{44} (C_{11} + 2/7 C_{12}) / ((C_{11} + 2C_{12})(C_{11} - C_{12})) = 1$

With the present values, we get A = 0.56.



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