MACROSCOPIC THEORY OF SECOND, THIRD, FOURTH AND FIFTH ORDER ELASTIC CONSTANTS OF CUBIC STRUCTURE SOLID

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ABSTRACT :

The macroscopic theory of elastic constants reported by Thurston and Bragger has been extended using the Piola-Kirchhoff stress tensor algebra to obtain the expression for the natural wave velocity in terms of second, third, fourth and fifth order elastic coupling coefficient.

Key words : Cubic structure solids , Elastic constants

INTRODUCTION :

The analysis of experimental data of anharmonic properties is complicated due to the fact that the vibrational contribution contains coupling parameters of higher order than the contribution from the binding energy of the solid. In the long wave limits (Continua approximation) the vibrational contributions can be evaluated from the higher order elastic constants[1-3] without the knowledge of the microscopy coupling parameters. As these higher order elastic constants are directly related to pressure derivatives of bulk and shear modulie[4-6] which are needeed in study of condensed matter physics, geophysical and geochemical theories[7-14] of the interior of earth. In this direction various theories have been proposed[15-20] to study the higher order elastic constants by using the different forms of the binding energy. However, all these studies generally are limited to explain the elastic constants upto the fourth order of cubic structure solids. Out of all above theories 15-20 the lattice theory[17] is more general and suitable as it can be used to explain the various physical properties of the cubic structure solids.

Originally Srinivasan[17] has developed a theory using the macroscopic theory of elasticity[21] and the lattice theory[22] to derive the general expression for TOE constants, piezo-elastic constants and strain optical constants of non primitive cubic structure solids using the pair potential form of the energy. This was further studied by Goyal et al.[23] by using the many body potential[24].

Later on Goyal and Kumar[25] extended the lattice theory[17] by using the many body potential and the extended macroscopic theory[26] to derive the experssions for the fourth order elastic constants of cubic structure solids. Now we are further extending the Srinivasan theory[17] to derive the expression for fifth order elatic constants of cubic structure solids. In the present study we are first extending the macroscopic theory earlier reported by Thurston and Bragger[21] and Kumar and Goyal[26] to derive the general expression for a natural wave velocity (W) which is available from experiments in terms of second, third, fourth and fifth order elastic constants. The deteil of the theory is given in the following section.

EQUATION OF MOTION :

Following the theory of mechanics of continua, the equation of motion of the material particle in a position in the absence of body forces in terms of Piola-Kirchoff stress tensor is given by :

$$\rho \ddot{x}_j = \frac{\partial}{\partial x_k} \tau_{kj} \qquad ...(1.1)$$

$$\tau_{kj} = \frac{1}{J} \frac{\partial x_k}{a_p} \frac{\partial x_j}{\partial a_j} t_{pq} \qquad ...(1.2)$$

where x_j is the coordinate of a particle in strained state a_p is the coordinate of a material particle in the unstrained state t_{pq}, is the second Piola-Kirchoff stress tensor, * be the stresses expressed in terms of Piola-Kirchoff stress tensor and J is the jacobian of the deformation and if related as

$$J = \frac{\rho_0}{\rho} = \frac{\partial x_k}{\partial a_p} \qquad ...(1.3)$$

where ρ is the density in the strain coordinate and ρ_0 is the density in the unstrain coordinate

On substituting τ_{kj} from equation (1.2) into equation (1.1) we have.

$$\rho \ddot{x}_j = \frac{\partial}{\partial x_k} \left\{ \frac{1}{J} \frac{\partial x_k}{\partial a_p} \right\} P_{jp} + \frac{1}{j} \frac{\partial x_k}{\partial a_p} \frac{\partial P_{jp}}{\partial x_k} \qquad ...(1.4)$$

The first Piola-Kirchoff stress tensor P_{jp} in equation of motion (1.4) is a function of the entropy and the deformation gradient as

$$P_{jp} = \left(\frac{\partial x_j}{\partial a_p} \right) t_{pq} \qquad ...(1.5)$$

where

$$t_{pq} = \rho_0 \left(\frac{\partial U}{\partial \eta_{pq}} \right)_s = \rho_0 \left(\frac{\partial F}{\partial \eta_{pq}} \right)_T \qquad ...(1.6)$$

here U and F are an internal and Helmholtz free energy per unit mass, η_{pq} is the Lagrangian strain, S and T denote entropy and temperature.

In view of eq. (1.3), the eq. (1.4) becomes as

$$\rho_0 \ddot{x}_j = \frac{\partial P_{jp}}{\partial a_p} \qquad ...(1.7)$$

ELASTIC WAVES IN STRAINED MEDIUM :

Considering the propagation of small amplitude elastic waves in a homogeneously deformed medium, we assume P_{jp} in eq. (1.7) as a function of the entropy and the deformation gradient $\partial x_k/\partial a_m$. To obtain the linearized equation of motion, we expand P_{jp} about the initial state of coordinates x_i, denoting the initial values by ~ over the symbols.

$$P_{jp} - \tilde{P}_{jp} = \tilde{A}^{s}_{jpkl}\frac{\partial u_k}{\partial a_m} + \frac{1}{2}\tilde{A}^{s}_{jpkmrs}\frac{\partial u_k}{\partial a_m}\frac{\partial u_r}{\partial a_s} + \tilde{A}^{s}_{jpkmrsld}\frac{\partial u_k}{\partial a_m}\frac{\partial u_r}{\partial a_s}\frac{\partial u_l}{\partial a_d} \quad ...(1.8)$$

where $u_i = x_i - X_i$ be the component of displacement from initial state due to the wave. X_i and X_i denotes coordinate in homogeneously final and initial state respectively.

$$\tilde{A}^{s}_{jpkm} = \frac{\partial P_{jp}}{\partial\left(\frac{\partial X_k}{\partial a_m}\right)}$$

$$\tilde{A}^{s}_{jpkmrs} = \frac{\partial^2 P_{jp}}{\partial\left(\frac{\partial X_k}{\partial a_m}\right)\partial\left(\frac{\partial x_r}{\partial a_s}\right)}$$

$$\tilde{A}^{s}_{jpkmrsld} = \frac{\partial^3 P_{jp}}{\partial\left(\frac{\partial X_k}{\partial a_m}\right)\partial\left(\frac{\partial x_r}{\partial a_s}\right)\partial\left(\frac{\partial x_i}{\partial a_d}\right)} \quad ...(1.9)$$

On substituting an eq. (1.8) into the eq. (1.7) and retaining upto third power's of the displacement gradients (□$u_k/\partial a_m$). ($\partial u_r/\partial a_s$). ($\partial u_l/\partial a_d$) we find the linearized equation of motion for u_j in the following forms.

$$P_0\ddot{u}_j = \tilde{A}^{s}_{jpkm}\frac{\partial^2 u_k}{\partial a_p a_m} + \frac{1}{2}\tilde{A}^{s}_{jpkmrs}\frac{\partial^2 u_k}{\partial a_p a_m}\frac{\partial u_r}{\partial a_s} + \frac{1}{6}\tilde{A}^{s}_{jpkmrsld}\frac{\partial^2 u_k}{\partial a_p a_m}\frac{\partial u_r}{\partial a_s}\frac{\partial u_l}{\partial a_d} \quad ...(1.10)$$

'A' COEFFICIENT :

With the help of an equation (1.5), an equation (1.9a) forthe tensor $\tilde{A}^{s}_{jpkm}$ can be expressed in terms of the deformation gradients.

$$\tilde{A}^{s}_{jpkm} = \frac{\partial\left(\frac{\partial x_j}{\partial a_p}\right)}{\partial\left(\frac{\partial X_k}{\partial a_m}\right)} t_{pq} + \frac{\partial x_j}{\partial a_q}\frac{\partial t}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)} \quad ...(1.11)$$

Using tensor algebra above equation (1.11) can be written as

$$\tilde{A}^{s}_{jpkm} = \frac{\delta_{jk} t_{pm} + \frac{\partial x_j}{\partial a_q} \frac{\partial t_{pq}}{\left(\frac{\partial x_k}{\partial a_m}\right)}}{} \quad ...(1.12)$$

using the definitions of Lagrangian strain and its derivatives.

$$\eta_{ij} = \frac{1}{2}\left(\frac{\partial x_k}{\partial a_i}\frac{\partial x_k}{\partial a_j} - \delta_{ij}\right) \quad ...(1.13)$$

$$\frac{\partial \eta_{ij}}{\partial\left(\frac{\partial x_k}{\partial a_q}\right)} = \frac{1}{2}\left(\frac{\partial x_k}{\partial a_i}\frac{\partial x_k}{a_j} - \delta_{ij}\right) \quad ...(1.14)$$

The 'A' coefficient in eq. (1.12) can be expressed with the help of an eq. (1.14) in terms of the deformation gradients and the derivatives of an internal energy with respect to the Lagrangian strain η_{ij} as

$$\tilde{A}^{s}_{jpkm} = \delta_{jk} t_{pm} + \frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_i} C^{s}_{pqmi} \quad ...(1.15)$$

Where

$$C^{s}_{pqmi} = \left(\frac{\partial t_{pq}}{\partial \eta_{mi}}\right)_s = \rho_0 \left(\frac{\partial^2 U}{\partial \eta_{pq} \partial \eta_{mi}}\right)_s \quad ...(1.16)$$

Similarly on putting the value of P_{jp} from an equation (1.5) into equation (1.9b) we get

$$\tilde{A}^{s}_{jpkmrs} = \frac{\partial\left(\frac{\partial x_j}{\partial a_q}\right)}{\partial\left(\frac{\partial x_r}{\partial a_s}\right)\partial\left(\frac{\partial x_k}{\partial a_m}\right)} t_{pq} + \frac{\partial\left(\frac{\partial x_j}{\partial a_q}\right)}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)\partial\left(\frac{\partial x_k}{\partial a_m}\right)} + \frac{\partial x_j}{\partial a_q}\frac{\partial^2 t_{pq}}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)\partial\left(\frac{\partial x_r}{\partial a_s}\right)}$$

...(1.17)

using tensor algebra above equation can be written as

$$\tilde{A}^{s}_{jpkmrs} = \delta^{j}_{r}\delta^{j}_{s}\delta^{q}_{m} t_{pq} + \delta^{l}_{k}\delta^{q}_{m}\frac{\partial t_{pq}}{\partial\left(\frac{\partial x_r}{\partial a_s}\right)} + \delta^{j}_{r}\delta^{p}_{s}\frac{\partial t_{pq}}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)} + \frac{\partial x_j}{\partial q_q}\frac{\partial^2 t_{pq}}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)\partial\left(\frac{\partial x_r}{\partial a_s}\right)}$$

...(1.18)

Now using equation (1.14) we can write (1.18) as

$$\tilde{A}^{s}_{jpkmrs} = \delta^{j}_{r}\delta^{j}_{s}\delta^{q}_{m} t_{pq} + \delta^{j}_{k}\delta^{q}_{m}\frac{\partial x_r}{\partial a_n} C^{s}_{pqsn}$$

$$+\delta^{j}_{r}\delta^{q}_{s}\frac{\partial x_k}{\partial a_i} C^{s}_{pqmi} + \frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_i}\frac{\partial x_r}{\partial a_n} C^{s}_{pqmisn} \quad ...(1.19)$$

Where

$$C^{s}_{pqmi} = \left(\frac{\partial t_{pq}}{\partial \eta_{mi}}\right)_s = \rho_0 \left(\frac{\partial^2 U}{\partial \eta_{pq} \partial \eta_{mi}}\right)_s$$

$$C^{s}_{pqsn} = \left(\frac{\partial t_{pq}}{\partial \eta_{sn}}\right)_s = \rho_0 \left(\frac{\partial^2 U}{\partial \eta_{pq} \partial \eta_{sn}}\right)_s$$

$$C^{s}_{pqmisn} = \left(\frac{\partial t_{pq}}{\partial \eta_{mi} \partial \eta_{sn}}\right)_s = \rho_0 \left(\frac{\partial^2 U}{\partial \eta_{pq} \partial \eta_{mi} \partial \eta_{sn}}\right)_s$$

...(1.20a-c)

Similarly putting the value of P_{jp} from an eq. (1.5) into equation (1.9c) we get

$$\tilde{A}^{s}_{jpkmrsld} = \frac{\partial^3 \left(\frac{\partial x_j}{\partial a_q}\right) t_{pq}}{\partial \left(\frac{\partial x_k}{\partial a_m}\right) \partial \left(\frac{\partial x_r}{\partial a_s}\right) \partial \left(\frac{\partial x_i}{\partial a_d}\right)}$$

$$\tilde{A}^{s}_{jpkmrsld} = \frac{\partial^3 \left(\frac{\partial x_j}{\partial a_q}\right) t_{pq}}{\partial \left(\frac{\partial x_r}{\partial a_s}\right) \partial \left(\frac{\partial x_k}{\partial a_m}\right) \partial \left(\frac{\partial x_i}{\partial a_d}\right)} + \frac{\partial \left(\frac{\partial x_j}{\partial a_q}\right) \partial^2 t_{pq}}{\partial \left(\frac{\partial x_r}{\partial a_s}\right) \partial \left(\frac{\partial x_l}{\partial a_d}\right) \partial \left(\frac{\partial x_k}{\partial a_m}\right)}$$

$$+ \frac{\partial \left(\frac{\partial x_j}{\partial a_q}\right) \partial^2 t_{pq}}{\partial \left(\frac{\partial x_r}{\partial a_s}\right) \partial \left(\frac{\partial x_l}{\partial a_d}\right) \partial \left(\frac{\partial x_k}{\partial a_m}\right)} + \frac{\partial \left(\frac{\partial x_j}{\partial a_q}\right) \partial^2 t_{pq}}{\partial \left(\frac{\partial x_l}{\partial a_d}\right) \partial \left(\frac{\partial x_r}{\partial a_s}\right) \partial \left(\frac{\partial x_k}{\partial a_m}\right)}$$

$$+ \frac{\partial t_{pq}}{\partial \left(\frac{\partial x_k}{\partial a_m}\right)} \frac{\partial^2 \left(\frac{\partial x_j}{\partial a_q}\right)}{\partial \left(\frac{\partial x_k}{\partial a_m}\right) \partial \left(\frac{\partial x_r}{\partial a_s}\right) \partial \left(\frac{\partial x_l}{\partial a_d}\right)} + \frac{\partial t_{pq}}{\partial \left(\frac{\partial x_r}{\partial a_s}\right)} \frac{\partial^2 \left(\frac{\partial x_j}{\partial a_q}\right)}{\partial \left(\frac{\partial x_k}{\partial a_m}\right) \partial \left(\frac{\partial x_l}{\partial a_d}\right)}$$

$$+ \frac{\partial t_{pq}}{\partial \left(\frac{\partial x_l}{\partial a_d}\right)} \frac{\partial^2 \left(\frac{\partial x_j}{\partial a_q}\right)}{\partial \left(\frac{\partial x_k}{\partial a_m}\right) \partial \left(\frac{\partial x_r}{\partial a_s}\right)} + \frac{\partial^2 t_{pq}}{\partial \left(\frac{\partial x_k}{\partial a_m}\right) \partial \left(\frac{\partial x_r}{\partial a_s}\right) \partial \left(\frac{\partial x_l}{\partial a_d}\right)} \quad ...(1.21)$$

using tensor algebra eq. (1.21) can be written as

$$\tilde{A}^{s}_{jpkmrsld} = \delta^j_r\delta^q_s\delta^q_k\delta^q_m\delta^j_l\delta^q_d t_{pq} + \delta^j_k\delta^q_m \frac{\partial^2 t_{pq}}{\partial\left(\frac{\partial x_r}{\partial a_s}\right)\partial\left(\frac{\partial x_l}{\partial a_d}\right)} + \delta^j_r\delta^q_s \frac{\partial^2 t_{pq}}{\partial\left(\frac{\partial x_l}{\partial a_d}\right)\partial\left(\frac{\partial x_k}{\partial a_m}\right)}$$

$$+\delta^j_l\delta^q_d \frac{\partial^2 t_{pq}}{\partial\left(\frac{\partial x_l}{\partial a_s}\right)\partial\left(\frac{\partial x_k}{\partial a_m}\right)} + \delta^j_r\delta^q_s\delta^j_l\delta^q_d \frac{\partial t_{pq}}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)} + \delta^j_k\delta^q_m\delta^j_l\delta^q_d \frac{\partial t_{pq}}{\partial\left(\frac{\partial x_r}{\partial a_s}\right)}$$

$$+\delta^j_k\delta^q_m\delta^j_r\delta^q_s \frac{\partial t_{pq}}{\partial\left(\frac{\partial x_l}{\partial a_d}\right)} + \frac{\partial x_j}{\partial a_q} \frac{\partial^3 t_{pq}}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)\partial\left(\frac{\partial x_r}{\partial a_s}\right)\partial\left(\frac{\partial x_l}{\partial a_d}\right)} \quad ...(1.22)$$

where

$$\partial\left(\frac{\partial x_j}{\partial a_q}\right) = \delta^j_q$$

$$\frac{\partial t_{pq}}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)} = C^s_{pqmi}\frac{\partial x_k}{\partial a_i}$$

$$\frac{\partial t_{pq}}{\partial\left(\frac{\partial x_l}{\partial a_d}\right)} = C^s_{pqdz}\frac{\partial x_l}{\partial a_z}$$

$$\frac{\partial t_{pq}}{\partial\left(\frac{\partial x_l}{\partial a_d}\right)} = C^s_{pqdz}\frac{\partial x_l}{\partial a_z}$$

$$\frac{\partial t^2_{pq}}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)\partial\left(\frac{\partial x_r}{\partial a_s}\right)} = \frac{\partial x_k}{\partial a_i}\frac{\partial x_r}{\partial a_n}C^s_{pqmisn}$$

$$\frac{\partial t^2_{pq}}{\partial\left(\frac{\partial x_r}{\partial a_s}\right)\partial\left(\frac{\partial x_l}{\partial a_d}\right)} = \frac{\partial x_r}{\partial a_n}.\frac{\partial x_l}{\partial a_z}C^s_{pqsndz}$$

$$\frac{\partial t^2_{pq}}{\partial\left(\frac{\partial x_l}{\partial a_d}\right)\partial\left(\frac{\partial x_k}{\partial a_m}\right)} = \frac{\partial x_l}{\partial a_z}.\frac{\partial x_k}{\partial a_i}C^s_{pqmidz}$$

$$\frac{\partial t^3_{pq}}{\partial\left(\frac{\partial x_k}{\partial a_m}\right)\partial\left(\frac{\partial x_r}{\partial a_s}\right)\partial\left(\frac{\partial x_l}{\partial a_d}\right)} = \frac{\partial x_k}{\partial a_i}.\frac{\partial x_r}{\partial a_n}.\frac{\partial x_l}{\partial a_z}C^s_{pqmisndz} \qquad ...(1.23)$$

Now using eq. (1.14) we can write eq. (1.23) as

$$\tilde{A}^s_{jpkmrsld} = \delta^j_k\delta^q_m\delta^j_r\delta^q_s\delta^j_l\delta^q_d t_{pq} + \delta^j_k\delta^q_m\frac{\partial x_r}{\partial a_n}.\frac{\partial x_l}{\partial a_z}C^s_{pqsndz} + \delta^j_r\delta^q_s\frac{\partial x_l}{\partial a_z}.\frac{\partial x_k}{\partial a_i}C^s_{pqmidz}$$

$$\tilde{A}^s_{jpkmrsld} = \delta^j_k\delta^q_m\delta^j_r\delta^q_s\delta^j_l\delta^q_d t_{pq} + \delta^j_k\delta^q_m\frac{\partial x_r}{\partial a_n}.\frac{\partial x_l}{\partial a_z}C^s_{pqsndz}$$
$$+\delta^j_r\delta^q_s\frac{\partial x_l}{\partial a_z}.\frac{\partial x_k}{\partial a_i}.\frac{\partial x_l}{\partial a_z}C^s_{pqmidz} + \delta^j_l\delta^q_d\frac{\partial x_r}{\partial a_n}.\frac{\partial x_k}{\partial a_i}C^s_{pqmisn}$$
$$+\delta^j_r\delta^q_s\delta^j_l\delta^q_d\frac{\partial x_k}{\partial a_i}C^s_{pqmi} + \delta^j_k\delta^q_m\delta^j_l\delta^q_d\frac{\partial x_r}{\partial a_n}C^s_{pqsn}$$
$$+\delta^j_k\delta^q_m\delta^j_r\delta^q_s\frac{\partial x_l}{\partial a_z}C^s_{pqdz} + \frac{\partial x_j}{\partial a_q}.\frac{\partial x_k}{\partial a_i}.\frac{\partial x_r}{\partial a_n}.\frac{\partial x_l}{\partial a_z}C^s_{pqmisndz} \qquad ...(1.24)$$

where

$$C^s_{pqmi} = \left(\frac{\partial t_{pq}}{\partial \eta_{mi}}\right)_s = \rho_0\left(\frac{\partial^2 U}{\partial\eta_{pq}\partial\eta_{mi}}\right)_s$$

$$C^s_{pqsn} = \left(\frac{\partial t_{pq}}{\partial \eta_{sn}}\right)_s = \rho_0\left(\frac{\partial^2 U}{\partial\eta_{pq}\partial\eta_{sn}}\right)_s$$

$$C^s_{pqmisn} = \left(\frac{\partial^2 t_{pq}}{\partial \eta_{mi}\partial\eta_{sn}}\right)_s = \rho_0\left(\frac{\partial^3 U}{\partial\eta_{pq}\partial\eta_{mi}\partial\eta_{sn}}\right)_s$$

$$C^s_{pqmidz} = \left(\frac{\partial^2 t_{pq}}{\partial \eta_{dz}\partial\eta_{mi}}\right)_s = \rho_0\left(\frac{\partial^3 U}{\partial\eta_{pq}\partial\eta_{dz}\partial\eta_{mi}}\right)_s$$

$$C^s_{pqsndz} = \left(\frac{\partial^2 t_{pq}}{\partial \eta_{sn}\partial\eta_{dz}}\right)_s = \rho_0\left(\frac{\partial^3 U}{\partial\eta_{pq}\partial\eta_{sn}\partial\eta_{dz}}\right)_s$$

$$C^{s}_{pqmisndz} = \left(\frac{\partial^3 t_{pq}}{\partial\eta_{mi}\partial\eta_{sn}\partial\eta_{dz}}\right)_s$$

$$= \rho_0\left(\frac{\partial^4 U}{\partial\eta_{pq}\partial\eta_{mi}\partial\eta_{sn}\partial\eta_{dz}}\right)_s \qquad ...(1.25)$$

ELASTIC COEFFICIENTS :

In order to find the elastic constants (C-coefficients), the strain energy U can be expanded about the state of zero strain as

$$\rho_0 U = \frac{1}{2}\sum_{jp,km}\bar{C}_{jp,km}\eta_{jp} + \eta_{km} + \frac{1}{6}\sum_{jp,km,rs}\bar{C}_{jp,km,rs}\eta_{jp}\eta_{km}\eta_{rs}$$

$$+\frac{1}{24}\sum_{jp,km,rs,ld}\bar{C}_{jp,km,rs,ld}\eta_{jp}\eta_{km}\eta_{rs}\eta_{ld}$$

$$+\frac{1}{120}\sum_{jp,km,rs,ld,uv}\bar{C}_{jp,km,rs,ld}\eta_{jp}\eta_{km}\eta_{rs}\eta_{ld}\eta_{uv} \qquad ...(1.26)$$

Now the equation (1.26) is used in order to get the explicit expressions for t_{pm}, C^{s}_{pqmi}, $C^{s}_{pqsn}, C^{s}_{pqmisn}, C^{s}_{pqdz}, C^{s}_{pqdzmi}, C^{s}_{pqsndz}$ and $C^{s}_{pqmisndz}$ for this purpose we have used the following symmetric condition

$jp \leftrightarrow km \leftrightarrow rs \leftrightarrow ld \leftrightarrow uv$ we get

$$t_{pm} = \delta_{jp}\left[\sum_{rs}\bar{C}_{jp}\eta_{rs} + \frac{1}{2}\sum_{rs}\bar{C}_{jp,km}\eta_{km}\eta_{rs} - \sum_{km,rs}\bar{C}_{jp,km,rs,ld}\eta_{km}\eta_{rs}\eta_{ld}\right.$$

$$\left. + \frac{1}{2}\sum_{km,rs,ld,uv}\bar{C}_{jp,km,rs,ld,uv}\eta_{km}\eta_{rs}\eta_{ld}\eta_{uv}\right] \qquad ...(1.27)$$

$$C^{s}_{pqmi} = \delta_{jp}\delta_{ki}\left[\bar{C}_{jp,km}\sum_{rs}\bar{C}_{jp,km}\eta_{rs} + \frac{1}{2}\sum_{rs,ld}\bar{C}_{jp,km,rs,ld}\eta_{rs}\eta_{ld}\right.$$

$$\left.\frac{1}{6}\sum_{rs,ld,uv}\bar{C}_{jp,km,rs,ld,uv}\eta_{rs}\eta_{ld}\eta_{uv}\right] \qquad ...(1.28)$$

$$C^{s}_{pqsn} = \delta_{jp}\delta_{ks}\delta_{mm}\left[\bar{C}_{jp,km}\sum_{rs}\bar{C}_{jp,km,rs}\eta_{rs} + \frac{1}{2}\sum_{rs,ld}\bar{C}_{jp,km,rs,ld}\eta_{rs}\eta_{ld}\right.$$

$$\frac{1}{6}\sum_{rs,ld,uv}\bar{C}_{jp,km,rs,ld,uv}\eta_{rs}\eta_{ld}\eta_{uv}\Bigg] \quad ...(1.29)$$

$$C^{s}_{pqdz} = \delta_{jp}\delta_{kd}\delta_{mz}\Bigg[\bar{C}_{jp,km}\sum_{rs}\bar{C}_{jp,km,rs}\eta_{rs} + \frac{1}{2}\sum_{rs,ld}\bar{C}_{jp,km,rs,ld}\eta_{rs}\eta_{ld}$$

$$\frac{1}{6}\sum_{rs,ld,uv}\bar{C}_{jp,km,rs,ld,uv}\eta_{rs}\eta_{ld}\eta_{uv}\Bigg] \quad ...(1.30)$$

$$C^{s}_{pqmisn} = \delta_{jp}\delta_{ki}\delta_{m}\Bigg[\bar{C}_{jp,km,rs}\sum_{rs}\bar{C}_{jp,km,rs,ld}\eta_{ld} + \sum_{ld,uv}\bar{C}_{jp,km,rs,ld,uv}\eta_{id}\eta_{uv}\Bigg] \quad ...(1.31)$$

$$C^{s}_{pqmidz} = \delta_{jp}\delta_{ki}\delta_{rd}\delta_{sz}\Bigg[\bar{C}_{jp,km,rs}\sum_{rs}\bar{C}_{jp,km,rs,ld}\eta_{ld} + \sum_{ld,uv}\bar{C}_{jp,km,rs,ld,uv}\eta_{id}\eta_{uv}\Bigg]$$

...(1.32)

$$C^{s}_{pqsndz} = \delta_{jp}\delta_{mn}\delta_{rd}\delta_{kz}\Bigg[\bar{C}_{jp,km,rs}\sum_{rs}\bar{C}_{jp,km,rs,ld}\eta_{ld} + \sum_{ld,uv}\bar{C}_{jp,km,rs,ld,uv}\eta_{id}\eta_{uv}\Bigg]$$

...(1.33)

$$C^{s}_{pqmisndz} = \delta_{jp}\delta_{ki}\delta_{m}\delta_{lz}\Bigg[\bar{C}_{jp,km,rs,ld}\sum_{uv}\bar{C}_{jp,km,rs,ld}\eta_{uv}\Bigg] \quad ...(1.34)$$

ELASTIC WAVE :

Now we assume plane sinusoidal waves in the form

$$U_j = A_j \exp\left[j\omega\left(t - \frac{N_i a_i}{w}\right)\right] \quad ...(1.35)$$

According to this expression, the wave front is a material plane which has unit normal N in the natural state and a wave front moves from the plane N.a = 0 at N.a = L_0 in time Lo/W. Thus W is the wave speed reffered to natural dimensions and we call it the natural velocity for propagation normal to a plane of natural normal N. Deriving the equation for natural wave velocity (W) from ultra-sonic experiment be

$$W = 2\ LoF \quad ...(1.36)$$

where F is repetition frequency

The substitution of an equation (1.35) into linearized equation of motion (1.10) provides the following propagation condition of the wave

$$\rho_0 W^2 u_j = \tilde{A}^{s}_{jpkm} N_p N_m u_k + \frac{1}{2}\tilde{A}^{s}_{jpkmrs} N_p N_m N_s u_k u_r$$

$$+\frac{1}{6}\tilde{A}^{s}_{jpkmrsld} N_p N_m N_s u_k u_r u_l$$

$$N_p = \frac{\partial}{\partial a_p}$$

$$N_m = \frac{\partial}{\partial a_m}$$

$$N_s = \frac{\partial}{\partial a_s}$$

$$N_d = \frac{\partial}{\partial a_d}$$

When ‘A’ coefficients are defined by equations (1.15) and (1.19).

On applying the symmetric conditions $j \leftrightarrow k, p \leftrightarrow m, j \leftrightarrow r$ (1.15), (1.19), (1.28) and (1.19a) became as

$$A_{(jp),[rs],(km)} = \delta_{jk}\delta_{qm}\frac{\partial x_r}{\partial a_n}C^s_{pqsn} \quad ...(1.39)$$

$$A_{(jp),[rs],(km)} = \delta^j_r\delta^q_s\delta^j_k t_{pq} + \delta^j_k\delta^q_m\frac{\partial x_r}{\partial a_n}C^s_{pqsn} + \delta^j_r\delta^q_s C^s_{pqmi}\frac{\partial x_k}{\partial a_i} + \frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_i}\frac{\partial x_r}{\partial a_n}C^s_{pqmisn}$$

$$A_{(jp),[rs](km)} = \delta_{jk}\delta_{qm}\frac{\partial x_r}{\partial a_n}C^s_{pqsn} + \frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_i}\frac{\partial x_r}{\partial a_n}C^s_{pqmisn} \quad ...(1.40)$$

$$A_{(jp),[rs],(ld),(km)} = \delta^j_k\delta^q_m\delta^j_r\delta^j_i\delta^q_d t_{pq} + \delta^i_k\delta^q_m\frac{\partial x_r}{\partial a_n}\frac{\partial x_l}{\partial a_z}C^s_{pqsndz} + \delta^j_r\delta^q_s\frac{\partial x_l}{\partial a_z}\frac{\partial x_k}{\partial a_i}C^s_{pqmidz}$$

$$+\delta^j_k\delta^q_m\delta^j_r\delta^q_s\frac{\partial x_l}{\partial a_z}C^s_{pqdz} + \frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_i}\frac{\partial x_r}{\partial a_n}\frac{\partial x_l}{\partial a_z}C^s_{pqmisndz} \quad ...(1.41)$$

$$A_{(jp),[rs](ld),(km)} = \delta^j_k\delta^q_m\frac{\partial x_r}{\partial a_n}\frac{\partial x_l}{\partial a_z}C^s_{pqsndz} + \delta^j_r\delta^q_s\frac{\partial x_l}{\partial a_r}\frac{\partial x_k}{\partial a_i}C^s_{pqmidz}$$

$$+\delta^j_r\delta^q_s\delta^j_l\delta^q_d\frac{\partial x_k}{\partial a_i}C^s_{pqmi} + \delta^j_k\delta^q_m\delta^j_r\delta^q_s\frac{\partial x_r}{\partial a_n}C^s_{pqsn}$$

$$+\delta^j_k\delta^q_m\delta^j_r\delta^q_s\frac{\partial x_l}{\partial a_z}C^s_{pqdz} + \frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_i}\frac{\partial x_r}{\partial a_n}\frac{\partial x_l}{\partial a_z}C^s_{pqmisndz} \quad ...(1.42)$$

$$A_{(jp),[rs],[ld],(km)} = \delta_{jk}\delta_{qm}\frac{\partial x_r}{\partial a_n}\frac{\partial x_l}{\partial a_z}C^s_{pqsndz} + \delta_{jr}\delta_{qs}\frac{\partial x_l}{\partial a_r}\frac{\partial x_k}{\partial a_i}C^s_{pqmidz}$$

$$+\delta_{jr}\delta_{qs}\delta_{ji}\delta_{qd}\frac{\partial x_k}{\partial a_i}C^s_{pqmi}+\delta_{jk}\delta_{qm}\delta_{ji}\delta_{qd}\frac{\partial x_r}{\partial a_n}C^s_{pqsn}$$

$$+\delta_{jk}\delta_{qm}\delta_{jr}\delta_{qs}\frac{\partial x_l}{\partial a_z}C^s_{pqdz}+\frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_l}\frac{\partial x_r}{\partial a_n}\frac{\partial x_l}{\partial a_z}C^s_{pqmisndz} \quad ...(1.43)$$

$$A_{(jp),[rs][ld],(km)} = \delta_{jk}\delta_{qm}\frac{\partial x_r}{\partial a_n}\frac{\partial x_l}{\partial a_z}C^s_{pqsndz}+\delta_{jk}\delta_{qm}\delta_{jr}\delta_{qs}\frac{\partial x_r}{\partial a_n}C^s_{pqsn}$$

$$+\delta_{jk}\delta_{qm}\delta_{jr}\delta_{qs}\frac{\partial x_l}{\partial a_z}C^s_{pqdz}+\frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_i}\frac{\partial x_r}{\partial a_n}\frac{\partial x_l}{\partial a_z}C^s_{pqmisndz} \quad ...(1.44)$$

On substituting the value of t_{pm} and C^s_{pqmi} after neglecting the second-order term of the Lagrangian from eq. (1.27), (1.28) and Using eq. (1.13) becomes as

$$A_{(jp),(km)} = \bar{C}_{jp,km}+\delta_{km}\sum_{km}\bar{C}_{np,km,rs}\eta_{rs}+\delta_{jk}\delta_{jp}\delta_{ki}(2\eta_{qi}+\delta_{qi})$$

$$(\bar{C}_{jp,km}+\sum_{rs}\bar{C}_{jp,km,rs}\eta_{rs}) \quad ...(1.45)$$

using the tensor algebra and neglecting the second-order of the Lagrangian in the eq. (1.47) we get

$$A_{(jp),(km)} = \bar{C}_{jp,km}+\delta_{km}\sum_{km}\bar{C}_{jp,km,rs}\eta_{rs}+2\delta_{qi}\bar{C}_{jp,km}\eta_{qi} \quad ...(1.46)$$

Now using the following symmetric conditions in the

jp ↔ km ↔ rs, j ↔ p, k ↔ m, r ↔ s, j ↔ m, q = i

above equation we get

$$A_{(jp),(km)} = \bar{C}_{jp,km}+\sum_{rs}[\bar{C}_{jp,km,rs}+\delta_{jk}\bar{C}_{pmrs}]_{rs}+\sum_{q}\bar{C}_{jp,mk}\in_{jp}+\sum_{q}\bar{C}_{pi,mq}\in_{kj}$$

...(1.47)

similarly on substituting the value of $\frac{\partial x_l}{\partial a_z}C^s_{pqsn}$ after neglecting the second-term of the Lagrangian from equation (1.29), C^s_{pqmisn} from equation (1.31) and (1.13), the equation (1.40) becomes as

$$A_{(jp),[rs],(km)} = \delta_{jk}\delta_{qm}\delta_{jq}\delta_{ks}\delta_{mn}J\left(\bar{C}_{jp,km}+\sum_{rs}\bar{C}_{jp,km,rs}\eta\right)$$

$$\delta_{jk}\delta_{jq}\delta_{ki}\delta_{m}J(2\eta_{qi}+\delta_{qi})\left(\bar{C}_{jp,km,rs}+\sum_{rs}\bar{C}_{jp,km,rs,ld}\eta_{ld}\right) \quad ...(1.48)$$

using the tensor algebra and neglecting the second order term of the Lagrangian in the above equation we have

$$A_{(jp),[rs],(km)} = J\delta_{sn}\left[\bar{C}_{jp,km} + \sum_{rs}\bar{C}_{jp,km,rs}\eta_{rs}\right]$$

$$+J\delta_{sn}\left[\bar{C}_{jp,km,rs} + \sum_{ld}\bar{C}_{jp,km,rs,ld}\eta_{ld} + 2\delta_{qi}\bar{C}_{jp,km,rs}\eta_{qi}\right] \quad ...(1.49)$$

Now using the following symmetric conditions in the

$Jp \leftrightarrow km \leftrightarrow rs \leftrightarrow ld, j \leftrightarrow p, k \leftrightarrow m, r \leftrightarrow s, l \leftrightarrow d, j \leftrightarrow m, q = i, n = r$

above equation we get

$$A_{(jp),[rs],(km)} = \bar{C}_{pm,rs}\delta_{jk} + \bar{C}_{jp,km,rs} + \sum_{ld}[\bar{C}_{jp,km,rd,ld} + \bar{C}_{jp,rs,ld}]\eta_{ld}$$

$$+\sum_{q}\bar{C}_{jp,mk,rs} \in_{jp} + \sum_{ld}[\bar{C}_{jp,kq,rs} \in_{kq}] \quad ...(1.50)$$

Now on subsitituting the value of C^{s}_{pqsn} after neglecting the second order term of the Lagrangian from equation (1.20), C^{s}_{pqsndz} from equation (1.33), $C^{s}_{pqmisndz}$ from equation (1.34) and using eq. (1.3) and (1.13) eq. (1.44) become as

$$A_{(np),[rs][ld],(km)} = \delta_{jk}\delta_{qm}\delta_{jq}\delta_{mn}\frac{\partial x_l}{\partial a_z}J\left[\bar{C}_{jp,km,rs} + \sum_{ld}\bar{C}_{jp,km,rs,ld}\eta_{ld}\right]$$

$$+\delta_{jk}\delta_{qm}\delta_{jl}\delta_{ks}\delta_{mn}\frac{\partial x_l}{\partial a_z}J\left[\bar{C}_{jp,km} + \sum_{ld}\bar{C}_{jp,km,rs}\eta_{rs}\right]$$

$$+\delta_q\delta_{ki}\delta_m\delta_{iz}\frac{\partial x_j}{\partial a_q}\frac{\partial x_k}{\partial a_i}\frac{\partial x_k}{\partial a_k}\frac{\partial x_l}{\partial a_z}J\left[\bar{C}_{jp,km,rs,ld} + \sum_{uv}\bar{C}_{jp,km,rs,ld,uv}\eta_{uv}\right] \quad ...(1.51)$$

$$A_{(jp),[rs][ld],(km)} = \delta_{jk}\delta_{qm}\delta_{jq}\delta_{mn}\delta_{ki}\frac{\partial x_l}{\partial a_z}J\left[\bar{C}_{jp,km,rs} + \sum_{ld}\bar{C}_{jp,km,rs,ld}\eta_{ld}\right]$$

$$+\delta_{jk}\delta_{qm}\delta_{ji}\delta_{qd}\delta_{jq}\delta_{ks}\delta_{mn}J\left[\bar{C}_{jp,km} + \sum_{ld}\bar{C}_{jp,km,rs}\eta_{rs}\right]$$

$$+\delta_{jq}\delta_{qm}\delta_m\delta_{iz}\delta_{jk}(2\eta_{qi} + \delta_{qi})\left[\bar{C}_{jp,km,rs,ld} + \sum_{rs}\bar{C}_{jp,km,rs,ld,uv}\eta_{uv}\right] \quad ...(152)$$

Using the tensor algebra and neglecting the second order term of the Lagrangian in the above equation we have

$$A_{(jp),[rs],[ld],(km)} = \delta_{rd}\delta_{nz}\frac{\partial x_l}{\partial a_z} J\left[\bar{C}_{jp,km,rs} + \sum_{ld}\bar{C}_{jp,km,rs,ld}\eta_{ld}\right]$$

$$+\delta_{ld}\delta_{jq}\delta_{sn} J\left[\bar{C}_{jp,km} + \sum_{ld}\bar{C}_{jp,km,rs}\eta_{rs}\right]$$

$$+\delta_{jq}\delta_{m}\delta_{ld}\left[\bar{C}_{jp,km,rs,ld} 2\eta_{qi} + \delta_{qi}\bar{C}_{jp,km,rs,ld} + \delta_{qi}\sum_{rs}\bar{C}_{jp,km,rs,ld,uv}\eta_{uv}\right] \quad ...(1.53)$$

Now using the following symmetries conditions in the above equation

Jp ↔ km ↔ rs ↔ ld ↔ uv,j ↔ p,k ↔ m,r ↔ s,l ↔ d,u ↔ v,l ↔ z,q = i,n = r

$$A_{(jp),[rs],[ld],(km)} = \bar{C}_{jp,km} + \bar{C}_{jp,km,rs} + \bar{C}_{jp,km,rs,ld}\delta_{jq}$$

$$\sum_{uv}[\bar{C}_{jp,km,rs} + \bar{C}_{jp,km,rs,ld} + \bar{C}_{jp,km,rs,ld,uv}]\eta_{uv}$$

$$+\sum_{q}\bar{C}_{jp,rs,ld,km} \in_{jq} + \sum_{q}\bar{C}_{jp,rs,ld,mq} \in_{kq} \quad ...(1.54)$$

On simplifying equation (1.54) we get

$$A_{(jp),[rs],[ld],(km)} = \bar{C}_{pm,rs} + \bar{C}_{pm,rs,ld} + \bar{C}_{jp,km,rs,ld}$$

$$\sum_{uv}[\bar{C}_{pl,md,uv}\delta_{jk}\delta_{rs} + \bar{C}_{pl,md,rs,uv} + \bar{C}_{jp,km,rs,ld,uv}]\eta_{uv}$$

$$+\sum_{q}\bar{C}_{jp,rs,ld,km} \in_{jq} + \sum_{q}\bar{C}_{jp,rs,ld,mq} \in_{kq} \quad ...(1.55)$$

CONCLUSION :

The present derived propagation condition of a plane wave (equation-1.38) along with the equations of elastic constants derived by using lattice theory given by Born-Huang[22] will be useful in deriving the expressions for up to the fifth order elastic constants of cubic structure solids are other related an harmonic properties of the solids.

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