Phonon Dispersion curve of Silicon Carbide

Nutan Kumari

Department of Physics,

B.R.A. Bihar University, Muzaffarpur.

Abstract : The valence force field model developed for the study of phonon dispersion relations between frequency and wave vector along with the symmetry directions of some tetrahedrally bonded binary compounds. Results for phonon dispersion curves of Silicon Carbide are presented in this work. Calculations of phonon dispersion curves for each crystal are done on the theoretical formulation for the elements of the dynamical matrix based on valence force field approximation.

Keywords :- Valence force field, Frequency, wave vector.

I. INTRODUCTION

Feldman et al[2] and Schneider and Kirby[5] have obtained phonon dispersion curves of -SiC-based on the existence of polytypes. The work of Ziomek and Pickar[4] on the infrared absorption spectrum of -SiC is in agreement with the frequency assignments of Pickar et al[4].

No experimental neutron and scattering results are available for β- SiC. Experimental values of the elastic constants are also not available for β- SiC.

II. METHODOLOGY

Calculations of phonon dispersion curves for Silicon carbide crystal are done on the theoretical formulation for the elements of the dynamical matrix based on valence force field approximation. The secular equation for the normal modes of vibration of the lattice is given by

$$\left| D_{\alpha\beta}\left(\begin{matrix}\vec{q}\\ \sigma\sigma'\end{matrix}\right) - \omega^2\delta_{\alpha\beta}\delta_{\sigma\sigma'} \right| = 0 \qquad \text{.....(1)}$$

Where $D_{\alpha\beta}\left(\begin{matrix}\vec{q}\\ \sigma\sigma'\end{matrix}\right)$ represent the elements of the dynamical matrix and ω is the angular frequency for the normal modes of vibration. $\delta_{\alpha\beta}$ and $\delta_{\sigma\sigma'}$ are kronecker delta functions. The element $D_{\alpha\beta}\left(\begin{matrix}\vec{q}\\ \sigma\sigma'\end{matrix}\right)$ in the present work consists of two terms:

$$D_{\alpha\beta}\left(\begin{matrix}\vec{q}\\ \sigma\sigma'\end{matrix}\right) = D^{R}_{\alpha\beta}\left(\begin{matrix}\vec{q}\\ \sigma\sigma'\end{matrix}\right) + D^{C}_{\alpha\beta}\left(\begin{matrix}\vec{q}\\ \sigma\sigma'\end{matrix}\right) \qquad \text{.....(2)}$$

The first and second terms in the R.H.S. of the equation (2) represents the short range non-coulomb repulsive interaction and coulomb interactions, respectively. Each of the term is a (6x6) matrix.

PHONON DISPERSION RELATIONS ALONG [100] SYMMETRY DIRECTION

The expression for the frequency of the longitudinal modes can be obtained in terms of the model parameters α, β_1,β_2,β_3 and charge parameter X given by

$$X = \frac{z^2e^2}{a^3}$$

The equation of frequency for the longitudinal optic (LO) as well as the longitudinal acoustic (LA) modes:

$$\omega_{LO}^2 = \frac{D_{XX}\left(\frac{\vec{q}}{11}\right)+D_{XX}\left(\frac{\vec{q}}{22}\right)}{2} + \frac{1}{2}\left[\left\{D_{XX}\left(\frac{\vec{q}}{11}\right) - D_{XX}\left(\frac{\vec{q}}{22}\right)\right\}^2 + 4D_{XX}\left(\frac{\vec{q}}{12}\right)D_{XX}^*\left(\frac{\vec{q}}{12}\right)\right]^{\frac{1}{2}} \quad \text{... ... ...(3)}$$

$$\omega_{LA}^2 = \frac{D_{XX}\left(\frac{\vec{q}}{11}\right)+D_{XX}\left(\frac{\vec{q}}{22}\right)}{2} - \frac{1}{2}\left[\left\{D_{XX}\left(\frac{\vec{q}}{11}\right) - D_{XX}\left(\frac{\vec{q}}{22}\right)\right\}^2 + 4D_{XX}\left(\frac{\vec{q}}{12}\right)D_{XX}^*\left(\frac{\vec{q}}{12}\right)\right]^{\frac{1}{2}} \quad \text{... ... ... (4)}$$

AT ZONE CENTRE(Γ)

The expression for phonon frequencies at Zone center (Γ) is as follows

$$\omega_{LO}^2 = \frac{4}{m}\frac{e^2}{a^3}\left[\frac{\alpha}{3} + \frac{4}{3}\beta_1 + \frac{4}{3}\beta_2 - \frac{4}{3}\beta_3 + \frac{2\pi z^2}{6}\right] \quad \text{.....(5)}$$

and

$$\omega_{LA}^2(\Gamma) = 0 \quad \text{.....(6)}$$

where m is the reduced mass defined by

$$\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2} \quad \text{..... (7)}$$

$(m_2 > m_1)$ and X is the charge parameter given by

$$X = \frac{Z^2 e^2}{a^3}$$

AT ZONE BOUNDARY (X)

The equations (3) and (4) reduce to the following expressions at the zone boundary

$$\omega_{LO}^2(X) = \frac{4}{m_1}\frac{e^2}{a^3}\left[\frac{\alpha}{3} + \frac{10}{3}\beta_1 - \frac{2}{3}\beta_3 + 0.5041Z^2\right] \quad \text{.....(8)}$$

and

$$\omega_{LA}^2(X) = \frac{4}{m_2}\frac{e^2}{a^3}\left[\frac{\alpha}{3} + \frac{10}{3}\beta_2 - \frac{2}{3}\beta_3 + 0.5041Z^2\right] \quad \text{.....(9)}$$

TRANSVERSE MODES

At zone centre

$$\omega_{TO}^2(\Gamma) = \frac{4}{m}\frac{e^2}{a^3}\left[\frac{\alpha}{3} + \frac{4}{3}\beta_1 + \frac{4}{3}\beta_2 - \frac{2}{3}\beta_3 - \frac{\pi z^2}{6}\right] \quad \text{.....(10)}$$

and

$$\omega_{TA}^2(\Gamma) = 0 \quad \text{.....(11)}$$

AT ZONE BOUNDARY (X)

The frequencies of transverse optic and transverse acoustic modes are given by

$$\omega_{TO}^2(X) = \frac{1}{2}(S_1 + S_2) + \frac{1}{2}[(S_1 + S_2)^2 + 4S_3]^{\frac{1}{2}} \quad \text{.....(12)}$$

$$\omega_{TA}^2(X) = \frac{1}{2}(S_1 + S_2) - \frac{1}{2}[(S_1 + S_2)^2 + 4S_3]^{\frac{1}{2}} \quad \text{.....(13)}$$

where,

$$S_1 = \frac{1}{m_1}\frac{e^2}{a^3}\left[\frac{4}{3}\alpha + \frac{16}{3}\beta_1 + \frac{4}{3}\beta_2 - \frac{2}{3}\beta_3 - 1.083Z^2\right]$$

$$S_2 = \frac{1}{m_2}\frac{e^2}{a^3}\left[\frac{4}{3}\alpha + \frac{4}{3}\beta_1 + \frac{16}{3}\beta_2 - \frac{2}{3}\beta_3 - 1.083Z^2\right]$$

$$S_3 = \frac{1}{m_1 m_2}\frac{e^2}{a^3}\left[\frac{4}{3}\alpha - \frac{8}{3}\beta_1 - \frac{8}{3}\beta_2 - \frac{2}{3}\beta_3 - 5.312Z^2\right]^2$$

PHONON DISPERSION RELATION ALONG [110] SYMMETRY DIRECTION

The frequencies of the longitudinal and transverse phonons are given by the following expressions:

LONGITUDINAL PHONON MODES

$$\omega_{LO}^2 = \frac{D_{XX}\left(\frac{\vec{q}}{11}\right)+D_{XY}\left(\frac{\vec{q}}{11}\right)}{2} + \frac{D_{XX}\left(\frac{\vec{q}}{22}\right)+D_{XY}\left(\frac{\vec{q}}{22}\right)}{2} + \frac{1}{2}\left[\left\{D_{XX}\left(\frac{\vec{q}}{11}\right) + D_{XY}\left(\frac{\vec{q}}{11}\right) - D_{XX}\left(\frac{\vec{q}}{22}\right) - D_{XY}\left(\frac{\vec{q}}{22}\right)\right\}^2 + 4\left|D_{XX}\left(\frac{\vec{q}}{12}\right)\right|^2 + 4\left|D_{XY}\left(\frac{\vec{q}}{12}\right)\right|^2 + 4D_{XX}^*\left(\frac{\vec{q}}{12}\right)D_{XY}\left(\frac{\vec{q}}{12}\right) + 4D_{XX}\left(\frac{\vec{q}}{12}\right)D_{XY}\left(\frac{\vec{q}}{12}\right)\right]^{\frac{1}{2}} \quad (14)$$

$$\omega_{LA}^2 = \frac{D_{XX}\left(\frac{\vec{q}}{11}\right)+D_{XY}\left(\frac{\vec{q}}{11}\right)}{2} + \frac{D_{XX}\left(\frac{\vec{q}}{22}\right)+D_{XY}\left(\frac{\vec{q}}{22}\right)}{2} - \frac{1}{2}\left[\left\{D_{XX}\left(\frac{\vec{q}}{11}\right) + D_{XY}\left(\frac{\vec{q}}{11}\right) - D_{XX}\left(\frac{\vec{q}}{22}\right) + D_{XY}\left(\frac{\vec{q}}{22}\right)\right\}^2 + 4\left|D_{XX}\left(\frac{\vec{q}}{12}\right)\right|^2 + 4\left|D_{XY}\left(\frac{\vec{q}}{12}\right)\right|^2 + 4D_{XX}^*\left(\frac{\vec{q}}{12}\right)D_{XY}\left(\frac{\vec{q}}{12}\right) + 4D_{XX}\left(\frac{\vec{q}}{12}\right)D_{XY}^*\left(\frac{\vec{q}}{12}\right)\right]^{\frac{1}{2}} \quad \text{.....(15)}$$

TRANSVERSE PHONON MODES

$$\omega_{TO_1}^2 = \frac{D_{XX}\left(\frac{\vec{q}}{11}\right)-D_{XY}\left(\frac{\vec{q}}{11}\right)}{2} + \frac{D_{XX}\left(\frac{\vec{q}}{22}\right)-D_{XY}\left(\frac{\vec{q}}{22}\right)}{2} + \frac{1}{2}\left[\left\{D_{XX}\left(\frac{\vec{q}}{11}\right) - D_{XY}\left(\frac{\vec{q}}{11}\right) - D_{XX}\left(\frac{\vec{q}}{22}\right) - D_{XY}\left(\frac{\vec{q}}{22}\right)\right\}^2 + 4\left|D_{XX}\left(\frac{\vec{q}}{12}\right)\right|^2 + 4\left|D_{XY}\left(\frac{\vec{q}}{12}\right)\right|^2 - 4D_{XX}^*\left(\frac{\vec{q}}{12}\right)D_{XY}\left(\frac{\vec{q}}{12}\right) - 4D_{XX}\left(\frac{\vec{q}}{12}\right)D_{XY}^*\left(\frac{\vec{q}}{12}\right)\right]^{\frac{1}{2}} \quad (16)$$

$$\omega_{TA_1}^2 = \frac{D_{XX}\left(\frac{\vec{q}}{11}\right)-D_{XY}\left(\frac{\vec{q}}{11}\right)}{2} + \frac{D_{XX}\left(\frac{\vec{q}}{22}\right)-D_{XY}\left(\frac{\vec{q}}{22}\right)}{2} - \frac{1}{2}\left[\left\{\left(D_{XX}\left(\frac{\vec{q}}{11}\right) - D_{XY}\left(\frac{\vec{q}}{11}\right)\right) - \left(D_{XX}\left(\frac{\vec{q}}{22}\right) - D_{XY}\left(\frac{\vec{q}}{22}\right)\right)\right\}^2 + 4\left|D_{XX}\left(\frac{\vec{q}}{12}\right)\right|^2 + 4\left|D_{XY}\left(\frac{\vec{q}}{12}\right)\right|^2 - 4D_{XX}^*\left(\frac{\vec{q}}{12}\right)D_{XY}\left(\frac{\vec{q}}{12}\right) - 4D_{XX}\left(\frac{\vec{q}}{12}\right)D_{XY}^*\left(\frac{\vec{q}}{12}\right)\right]^{\frac{1}{2}} \quad (17)$$

$$\omega_{TO_2}^2 = \frac{D_{ZZ}\left(\frac{\vec{q}}{11}\right)+D_{ZZ}\left(\frac{\vec{q}}{22}\right)}{2} + \frac{1}{2}\left[\left\{D_{ZZ}\left(\frac{\vec{q}}{11}\right) - D_{ZZ}\left(\frac{\vec{q}}{22}\right)\right\} + 4\left|D_{ZZ}\left(\frac{\vec{q}}{12}\right)\right|^2\right]^{\frac{1}{2}} \quad \text{.....(18)}$$

and

$$\omega_{TA_2}^2 = \frac{D_{ZZ}\left(\frac{\vec{q}}{11}\right)+D_{ZZ}\left(\frac{\vec{q}}{22}\right)}{2} - \frac{1}{2}\left[\left\{D_{ZZ}\left(\frac{\vec{q}}{11}\right) - D_{ZZ}\left(\frac{\vec{q}}{22}\right)\right\}^2 + 4\left|D_{ZZ}\left(\frac{\vec{q}}{12}\right)\right|^2\right]^{\frac{1}{2}} \quad \text{.....(19)}$$

III. Results and Discussion

No experimental neutron and scattering results are available for β-SiC. Experimental values of the elastic constants are also not available for β-SiC. The theoretical values of the elastic constants C_{11}, C_{12}, C_{44} are reported by Tolpygo[6]. In the present work the theoretical values of elastic constants and phonon frequencies obtained from the Raman scattering experiment at the zone center and zone boundary

Table-1: Physical quantities used as input data and values of UVFF model parameters for SIC

Input data		
Macroscopic Physical Data	**Frequencies of Critical point phonon in units of 10^{12} cps**	**Calculated values of parameter in units of $a^3/e^2 \times 10^3$ dyne cm^{-1}**
C_{11}=35.23 ×10^{11} dyne cm^{-2}	ν_{LO} (Γ) = 29.14	α = 319.1938
C_{12}=14.04 ×10^{11} dyne cm^{-2}	ν_{TO} (Γ) = 23.86	β_1 = 7.1517
C_{44}=23.29 ×10^{11} dyne cm^{-2}	ν_{LO} (x) = 24.86	β_2 = 21.4560
2a = 4.348 ×10^{-8} cm	ν_{LA} (x) = 19.20	β_3 = 81.0294
m_1=19.7684 ×10^{-24} gm	ν_{TO} (x) = 22.83	X= 24.460
m_2 =46.2361 ×10^{-24} gm	ν_{TA} (x) = 11.19	

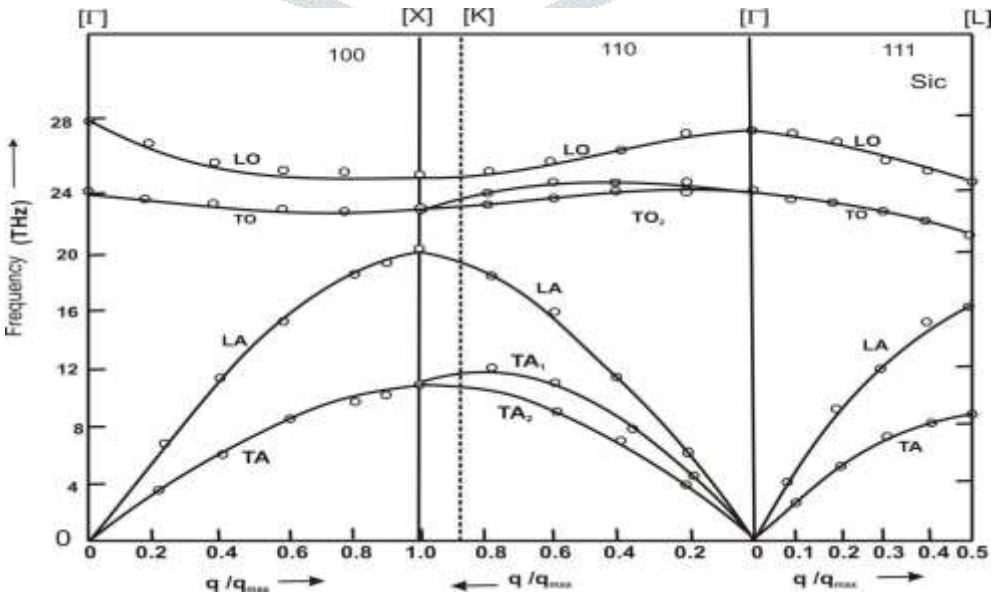

Fig-1 : Phonon dispersion curves of silicon carbide along symmetry directions. Circles are the experimental results

[100] direction has been used to obtain the model parameters. The input physical data and the values of model parameters are shown in table 1. calculated values of model parameters are used to calculate the phonon dispersion curves along [100], [111], and [110] symmetry directions in reciprocal space. These calculated curves with the available optical results are shown in Fig. 3.1. From the figure, it is clear that the calculated results are in good agreement with optical results.

Vetelino and Mitra[3] and Banerjee and Varshni[8] have presented results for β-SiC based on the model due to Rajagopal and Srinivasan[1] and the second neighbor rigid ion (SNI) model. Both models are rigid ion type models. The study of this compound has been also made with the help of shell model[10]. The lattice dynamic and thermodynamical properties of silicon carbideβ-SiC and other zinc blende type compounds have been also studied by Kunc and Balkanski[7] on the basis of the deformable bond approximation model. Since neutron scattering data and the experimental values of elastic constants are not available the reliability of the calculated results of phonon dispersion is yet to be tested.

IV. CONCLUSION

The study of the lattice vibrations of zinc-blende crystals has been undertaken on the basis of a phenomenological model that involves a reasonable small number of parameters. In the present work a rigid ion model utilizing valence force field approximation is developed for the lattice dynamics of zinc-blende compounds. The model developed involves only five disposable parameters and satisfies the condition of invariance of a lattice under rigid body rotation. The evaluation of force parameters does not require the extensive use of experimental phonon data. The valence force field model developed in the present work is employed to obtain the phonon dispersion curves of Silicon Carbide (SiC). The theoretical results obtained to explain the experimental values of phonon dispersion curves satisfactorily. Our results are more satisfactory compared to other theoretical predictions having a large number of model parameters which are evaluated employing experimental phonon frequencies.

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