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Many Body Interactions on Lattice Dynamical Properties of Stanene, 2D Material

Kamlesh Kumar[1], M. Imran Aziz[2], Nafis Ahmad[3]

[1,2]Physics Department, Shibli National Postgraduate College, Azamgarh, V.B.S.P. University, Jaunpur, Uttar Pradesh, India

[3]Mathematics Department, Shibli National Postgraduate College, Azamgarh, V.B.S.P. University, Jaunpur, Uttar Pradesh, India

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ABSTRACT

The study of the lattice dynamical properties of materials, phenomenological models describe a complete and straight forward description of the phonon dispersion and phonon eigenvectors in whole Brillouin Zone (BZ) and can be easily applied to the calculation of phonon density of states, elastic constants , dielectric permittivity and other properties of solid .Adiabatic Bond Charge Model (ABCM) was originally developed by W. Weber for studying the lattice dynamics of tetrahedrally bonded bulk group IV Semiconductors such as Si, Ge,Sn and diamond. The result obtained from this model is good agreement with the experimental data for Stanene. We, at present find the lattice dynamical matrix and secular equations using Adiabatic Bond Charge Model. We hope that lattice dynamical properties of Stanene as a 2D material will be good fitted with experimental data.

Keywords : Many body interactions, Adiabatic Bond Charge Model, Lattice dynamics of Stanene as 2D material.

I. INTRODUCTION

The experimental and theoretical studies on grapheme created significant interest in on other Group IV elements, compound of III-V and II-VI Group compound 2D nanostructures. Very recently, we have reported that among Group IV elements, not only C but also Si, Ge and Sn can form stable honeycomb structures [4, 5].The adiabatic bond charge (BCM) method was originally developed by Weber [3] in 1976. For studying the lattice dynamics of tetrahedrally bonded bulk group- IV semi conductors such as Silicon Germanium and Diamond. The model was also adapted by Rustagi and Weber for studying III- V Semiconductor [4] such as Gallium Arsenide. In Weber's approach the atom is considered a non- polarizable ion Core and a shell of Valence electrons. The Valence Charge density is considered as point charges, called bond charges which are located midway (For homopolar case) along the tetrahedral bonds between the nearest neighbors, whereas for (hetero polar) III-V semiconductors they

are nearer to the anions. These bond Charges are allowed to move adiabatically and are assumed to have zero mass. The equations of motion for the ions and their bond charges are evaluated and a dynamical matrix is obtained by considering three type of Interaction (i) Coulomb interactions (ii) Short range central force Interactions and (iii) a rotationally invariant Keating type bond bending Interaction depending on angle. These interactions are depicted in fig.(1)

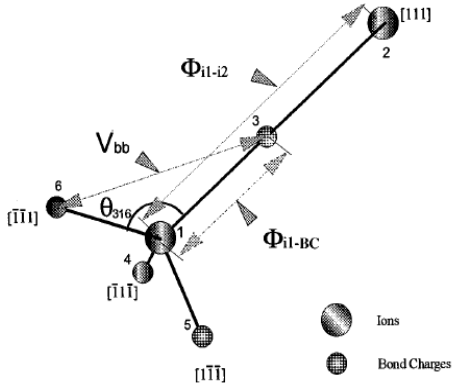
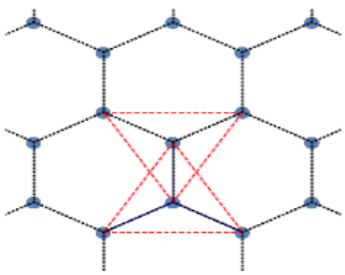


Fig . 1. Structure of unit cell and the interactions in the bond-charge model

Metal-like bonding is represented by the short-range central forces between ions (Φ_{i1-i2}) and covalent bonding is represented by the with cations and anions, and form interaction (c) there are different force constants associated with the BC-cation-BC and BC-anion-BC angles Keating interactions between the BC's (V_{bb}).For interaction (b) there are separate terms due to the interactions of the bond charges.

II. Modified Adiabatic bond Charge Model

The two-dimensional honeycomb lattice (Fig. 2) is



a triangular Bravais lattice with a two-point basis. It is defined by a set of primitive vectors, e.g. $a_1 = \sqrt{3}a(1, 0)$, and $a_2 = (\sqrt{3}/2)a(1,\sqrt{3})$, along with the positions of the atoms within each primitive cell, $c_1 = (0, 0)$, and $c_2 = a(0, 1)$. The length of each bond in the lattice is *a*. The position vector R of the lattice point is given as

$R=n_1a_1+n_2a_2$ …….

Where a_1 and a_2 are the independent primitive translational vectors and n_1, n_2 are integers.

Reciprocal lattice vectors are defined as

$$a_i b_j = 2\Pi\delta_{ij} \qquad \text{….. …..(2)}$$

The honeycomb 2D structure contains two ions and three BCs. Thus the magnitude of BCs is -2Ze and +3ze magnitude of ions due to neutrality of crystals. According to adiabatic bond charge model ,ther are three type of Interactions (i) Coulomb interactions (ii) Short range central force Interactions and (iii) a rotationally invariant Keating type bond bending Interaction depending on angle.In calculation of total potential energy,we added the zero point energy[5-6]. Moreover, with a finite nanocrystal, the Ewald transformation cannot be applied anymore but finite summations have to be computed. Thus the madelung constant α_m is replaced by α_m^{eff} which is given by

$$\alpha_m^{eff} = -\frac{r_0}{4}.\frac{1}{2}\sum_{ij}\frac{\zeta_i\zeta_j}{R^j - R^i} \qquad \text{….. …….(3)}$$

The total energy per unit cell of honeycomb structure is

$$\Phi_{total} = 3\left[\phi_{ii}(t)+\phi_1(r_1)+\phi_2(r_2)\right]-\alpha^{eff}{}_M\frac{(3Z)^2e^2}{\varepsilon t}+3\left[V_{bb}^1+V_{bb}^2+\psi_1(r^1{}_{bb})+\psi_2(r^2{}_{bb})\right]+\frac{1}{2}\hbar w_j(q)$$

…..(4)

In homopolar crystal $\Phi_1(r_1)=\Phi_2(r_2)$ and $V_{bb}^1=V_{bb}^2$. In addition, the ions and the BCs interact via the Coulomb interaction characterized by single parameter Z^2/ε where -2Ze is the charge of BC, and ε is the dielectric constant.

To reduce the number of parameters it is assumed that

$\psi_1' = \psi_2' = 0$, $\psi'' = -\psi'' = (B_2 - B_2)/8$ and $(1+p)\Phi_1' + (1-p)\Phi_2' = 0$ along the conditions for minimization of total energy per unit cell, which are $\left(\frac{\partial \Phi}{\partial t}\right)_0 = 0$ and $\left(\frac{\partial \Phi}{\partial p}\right)_0 = 0$ leads to

$$\phi_{ii}' = -\alpha_m \frac{Z^2}{\varepsilon}\frac{e^2}{t}$$

$$\frac{\phi_1'}{r_1} = 2\frac{d\alpha_m}{dp}\frac{1-p}{1+p}\frac{Z^2}{\varepsilon}\frac{e^2}{t^3} \quad \text{.....(5)}$$

$$\frac{\phi_2'}{r_2} = -2\frac{d\alpha_m}{dp}\frac{1+p}{1-p}\frac{z^2}{\varepsilon}\frac{e^2}{t^3}$$

The six parameters of the model are $\phi_{ii}'', \phi_1'', \phi_2'', B_1, B_2,$ and z^2/ε (Four for homopolar crystal).

The Fourier transformed of modified adiabatic bond Charge Model equations of motion

$$m\omega^2 u = \left[R + 9\frac{(Ze)^2}{\varepsilon}C_R\right]u + \left[T - 6\frac{(Ze)^2}{\varepsilon}C_T\right]v \ldots\ldots$$

$$0 = \left[T^+ - 6\frac{(Ze)^2}{\varepsilon}C_{T^+}\right]u + \left[S + 4\frac{(Ze)^2}{\varepsilon}C_S\right]v \ldots\ldots..$$

The above equations the $D_{\alpha\beta}(kk';q)$ can be reduced the ions the bond charge move adiabatically this gives

$$D^{eff} = D^{ion-ion} - \left[D^{BC-ion}\right]^*\left[D^{BC-BC}\right]^{-1}\left[D^{BC-ion}\right]$$

Where the D,s are those parts of the dynamical matrix referenced by their superscript and * denotes Hermitian conjugates. The condition for the non-trival solutions for wave amplitudes of Eq. 6 lead to the characteristic or secular equation;

$$\left|D^{eff}(q) - \omega^2(q)mI\right| = 0$$

$$\omega = \omega_j(q);\ j = 1,2,3,\ldots.2n$$

This is the secular relation.

III. Conclusion

Two-dimensional (2D) materials are one of the most active areas of nanomaterials research due to their potential for integration into next-generation electronic and energy conversion devices. Graphene, the most widely studied 2D material. Recently, the other 2D group-IV materials, silicene, germanene and stanene, have been realized by epitaxial growth on substrates [1-2], and attracted tremendous interest due to their extraordinary properties. The atoms in a solid are executing oscillations about their equilibrium positions with energy governed by the temperature of the solid .Such oscillations in crystals are called lattice vibrations. The lattice vibrations are responsible for the characteristic properties of matter such as specific heat, thermal conductivity, electrical conductivity, optical, elastic, dielectric properties, diffusion mechanism, phase change phenomena etc. The vibration of the atoms depends on the interatomic interaction within the crystal. To determine the vibrational frequencies and the corresponding modes one needs to calculate the eigenvalues and the eigenvectors of the so-called dynamical matrix, which can be obtained from the interatomic interactions potential [7-10]. If the dynamical matrix is known, the eigenvalue problem is straightforward. The use of phenomenological models in the study of the vibrational properties of IV group of semiconductor 2D material especially Stanene provides a complete and straightforward description of the phonon dispersion and phonon eigenvectors in the whole Brillouin Zone (BZ) with clear physical ingredients and a small computational effort.

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