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Effect of Many Body Interactions on Phonon Group Velocities of Stanene

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Abstract: 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. The discovery of stanene, a buckled monolayer of tin atoms arranged in a 2d honeycomb lattice, has explored enormous research interest in the materials in the two-dimensional (2D) realm. Stanene exhibit ductile nature and hence could be easily incorporated with existing technology in semiconductor industry on substrates in comparison to Graphene. The systematic investigation of phonon group velocities is needed for complete theoretical analysis of thermal energy transportandthermal conductivity of Stanene. The general three dimensional continuum model of phonons in two dimensional materials is developed for the theoretical prediction of the important thermal properties. The acoustical and optical contributions to the phonon group velocities are evaluated within the framework of Bond Charge Model. We, at present find the Phonon group velocities along symmetry directions using Adiabatic Bond Charge Model with the help of PYTHON Program. We hope that phonon group velocities along Γ–M of Stanene, 2D materials will have reasonably similar result obtained by other researchers.

Keywords: Many Body Interactions, Adiabatic Bond Charge Model, Phonon, Group Velocity, Stanene as a 2D Material

1. Introduction

Recently, the other 2D group-IV materials, Stanene, have been realized by epitaxial growth on substrates [1-2]. 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 eigenvalues problem is straightforward. There have been several theoretical attempts

to understand the lattice vibrations and Phonon properties of Stanene [11-13] usually employing the force constant model, the rigid ion model, the rigid shell model, the dipole approximation etc, but bond charge model is showing best results for IV th group of semiconductor. 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 figure 1.
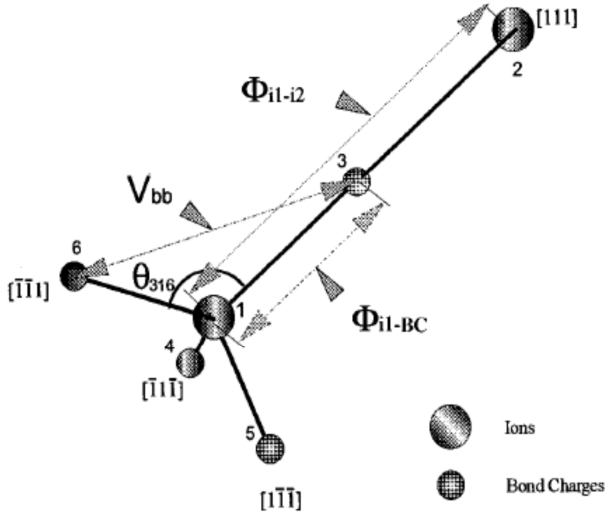

Figure 1. Structure of unit cell and the interactions in the bond-charge model.

Metal-like bonding is represented by the short-range central forces between ions $\left(\boldsymbol{\Phi}_{i1-i2}\right)$ 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.

2. Modified Adiabatic Bond Charge Model
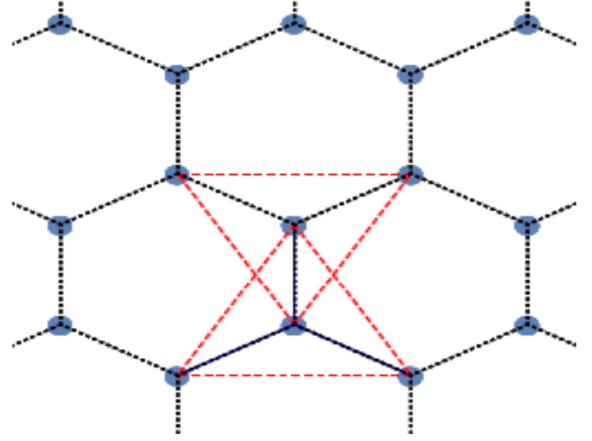
The two-dimensional honeycomb lattice (Figure 2) is

Figure 2. Stanene Lattice.

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, there 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.

The total energy per unit cell of honeycomb structure is

$$\Phi_{total} = 3\left[\boldsymbol{\varphi}_{ii}(t) + \boldsymbol{\varphi}_{1}(r_1) + \boldsymbol{\varphi}_{2}(r_2)\right] - \boldsymbol{\alpha}^{eff}_{M} \frac{(3Z)^2 e^2}{\varepsilon t} + 3\left[V^{1}_{bb} + V^{2}_{bb} + \boldsymbol{\psi}_{1}\left(r^{1}_{bb}\right) + \boldsymbol{\psi}_{2}\left(r^{2}_{bb}\right)\right] + \frac{1}{2}hw_j(q) \quad (1)$$

In homopolar crystal $\Phi_1(r_1) = \Phi_2(r_2)$ and $V^1_{bb} = V^2_{bb}$. 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

$\psi'_1 = \psi'_2 \quad = 0, \qquad \psi'' = -\psi'' = (B_2 - B_2)/8$ 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

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

$$\frac{\varphi'_1}{r_1} = 2\frac{d\alpha_m}{dp}\frac{1-p}{1+p}\frac{Z^2}{\varepsilon}\frac{e^2}{t^3} \quad (2)$$

$$\frac{\varphi'_2}{r_2} = -2\frac{d\alpha_m}{dp}\frac{1+p}{1-p}\frac{z^2}{\varepsilon}\frac{e^2}{t^3}$$

The six parameters of the model are $\boldsymbol{\varphi}''_{ii}, \varphi''_1, \varphi''_2, B_1, B_2,$ and z^2/ε (Four for homopolar crystal).

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

$$m\omega^2 u = \left[R + 9\frac{(Ze)^2}{\varepsilon} C_R \right] u + \left[T - 6\frac{(Ze)^2}{\varepsilon} C_T \right] v \quad (3)$$

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

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^{eff} 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. 3 lead to the characteristic or secular equation,

$$\left| D^{eff}(q) - \omega^2(q) mI \right| = 0 \quad (4)$$

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

This is the secular equation of 2x2 dimensions. Further it can be further extended as

$$-\omega^2 m_1 U = [D(0,0) - +D(0,1)D(1,1)^{-1}D(1,0)]U$$

where

$$D(0,0) = \begin{pmatrix} D_{xx}(0,0) & D_{xy}(0,0) \\ D_{yx}(0,0) & D_{yy}(0,0) \end{pmatrix}$$

$$D(1,0) = \begin{pmatrix} D_{xx}(1,0) & D_{xy}(1,0) \\ D_{yx}(1,0) & D_{yy}(1,0) \end{pmatrix}$$

$$D(0,1) = \begin{pmatrix} D_{xx}(0,1) & D_{xy}(0,1) \\ D_{yx}(0,1) & D_{yy}(0,1) \end{pmatrix}$$

$$D(1,1) = \begin{pmatrix} D_{xx}(1,1) & D_{xy}(1,1) \\ D_{yx}(1,1) & D_{yy}(1,1) \end{pmatrix}$$

The elements of dynamical matrix are defined as

$$D_{\alpha\beta}\left(\frac{kk'}{q}\right) = \sum_{l'} \Phi_{\alpha\beta}(l'-l;kk')exp\,(iq.r(lk,l'k')) \quad (5)$$

The above equation in matrix form is solved by Python program. And the result is obtained along hexagonal Brillouin zone with symmetry points $\Gamma(0,0)$. $M(0,\frac{2\pi}{a\sqrt{3}})$ and $K(2\pi/3a, \frac{2\pi}{a\sqrt{3}})$

The dispersion relations along symmetry line $\Gamma - M$ with coupling constant $\gamma_{j=8.4 \times 10^{-3}}\gamma$ for stanene is

$$\omega_1^2 = \gamma_j \left[1 - \cos\left(\frac{\sqrt{3}}{2} q_y a\right) \right]$$

$$\omega_2^2 = 3\gamma_j \left[1 - \cos\left(\frac{\sqrt{3}}{2} q_y a\right) \right]$$

$$\omega_3^2 = \left[\frac{3}{2} \gamma_j - \left(\frac{5}{4}\right) \gamma_j - \gamma_j \cos\left(\frac{\sqrt{3}}{2} q_x a\right) \right] \quad (6)$$

$$\omega_4^2 = \left[\frac{3}{2} \gamma_j + \left(\frac{5}{4}\right) \gamma_j + \gamma_j \cos\left(\frac{\sqrt{3}}{2} q_x a\right) \right]$$

$$\omega_5^2 = 0$$

$$\omega_6^2 = 3\gamma_j$$

Phonon group velocity.

$$v_g = \frac{d\omega_j}{dq_j}$$

$$q_j = q_x, q_x$$

$$v_{s1} = \frac{\sqrt{3}}{4} a(\gamma_j)^{\frac{1}{2}} \left[\cos\left(\frac{\sqrt{3}}{4} q_y a\right) \right]$$

$$v_{s2} = a\left(\frac{9}{8}\gamma_j\right)^{\frac{1}{2}} \left[\cos\left(\frac{\sqrt{3}}{4} q_y a\right) \right]$$

$$v_{s3} = \frac{\sqrt{3}}{2} a(\gamma_j)^{\frac{1}{2}} \left[\sin\left(\frac{\sqrt{3}}{2} q_x a\right) + \sin(\sqrt{3} q_x a) \right] \quad (7)$$

$$v_{s4} = 0$$

$$v_{s5} = 0$$

$$v_{s6} = -\frac{\sqrt{3}}{2} a(11\gamma_j)^{\frac{1}{2}} \left[\sin\left(\frac{\sqrt{3}}{2} q_x a\right) - \sin(\sqrt{3} q_x a) \right]$$

The phonon group velocities have been computed by solving the secular equation for the six vibration frequencies corresponding to the phonon wave vectors along the principal symmetry direction $\Gamma - M$ with the help of Python Program [Appendix 1]. There exists number of phonon branches such as LA, TA, ZA, LO, TO, ZO in Stanene [20] Their existence can be explained by the quantization of lattice waves along the X-Y axis due to partial or complete phonon spatial confinement along the cross-plane direction. Figure 3 shows the group velocities for Stanene. The observations inferred from this figure are as follows, six curves show the group velocity corresponding to six phonon branches. The six peaks are 28.696 cm^{-1}, 46.957 cm^{-1}, 104.348 cm^{-1}, 132.174 cm^{-1}, 150.435 cm^{-1}, 172.174 cm^{-1} has been observed in phonon density of states [20]. The group velocity has been reduced in the nanostructure due to complete phonon confinement. Group velocity approaches to zero as wave vector approaches to zero. Some phonon branches have more group velocity as compared to bulk. No phonon branch has velocity more than that in bulk cladding material. Along the principal symmetry direction $\Gamma - M$, 1750–6600 m/s, sound velocities are found in Stanene. Stanene is very important from device point of view. In general flow of electrons is impeded by the presence of phonons. More particularly heating of the interfaces would also be avoided in the application of the Stanene for the devices. The dispersion of phonon is helpful in understanding the heat evolution and transmission in 2D materials. The phonon dispersion relations for Stanene has been plotted and utilized to study the phonon group velocities in these structures. The affect of phonon confinement on the two

structures is different. Group velocity is suppressed in one case and enhanced in the other. Figure 3 shows that the variation of ω with k is linear for bulk (shown by dotted line). On the other hand in Stanene variation of V_g with q is anomalous which has also been shown in the same figure (curved lines). There is considerable decrease in group velocity from its bulk value. The reduced group velocity will result in reduced thermal conductivity. This result has also been corroborated by Bo Peng *et al.* [17]. Firstly, some phonon branches exhibits relatively more slopes. Secondly, the cut-off frequency is lowered for each branch. Such difference exists due to different types of phonon confinement in these two structures. Group velocity for some branches has been increased not only from there free standing value, but also from their bulk value. We derived the solution for the Γ and M points and numerically investigated the buckling effect on the material for phonon properties. We mainly fitted our model to account for the phonon group velocities. Our Bond Charge Model provides a reasonable good match for the high symmetry point's Γ, M and it is suitable for the study of the phonon group velocity of Stanene at various symmetry points [14-16].
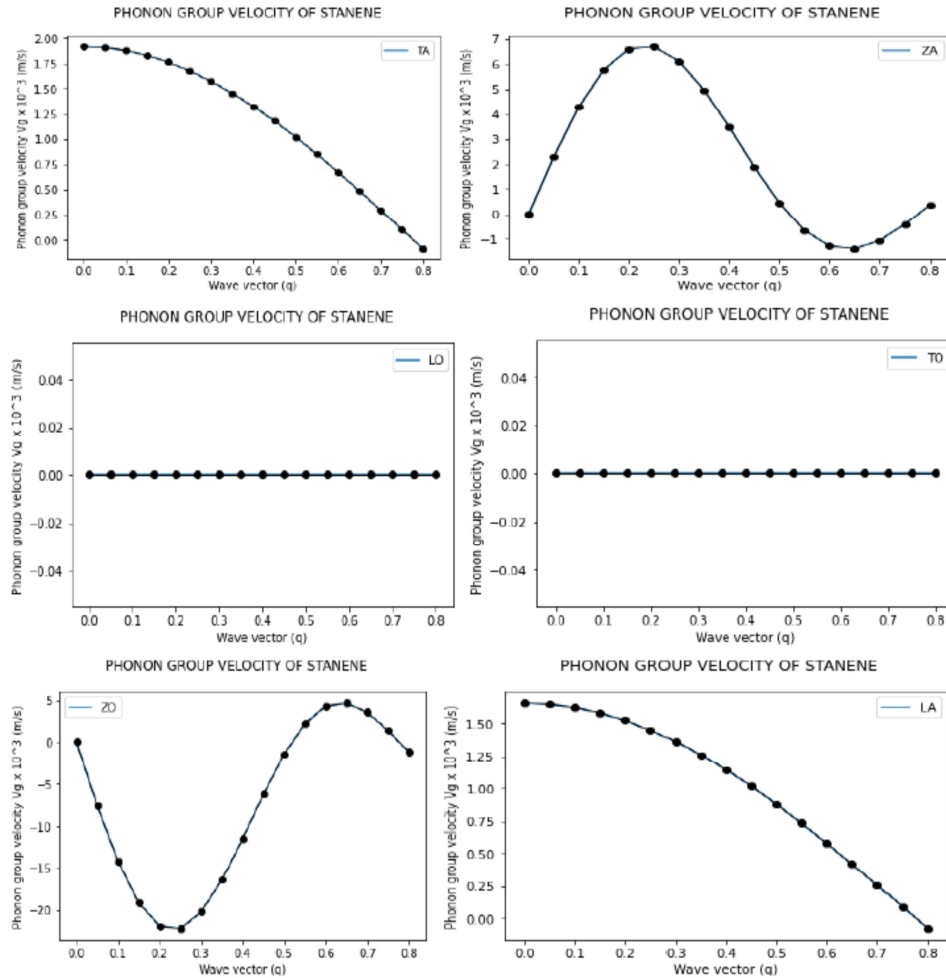

Figure 3. Calculated Phonon group velocities for Stanene along symmetry line Γ- M.

3. Conclusion

The use of phenomenological models in the study of the phonon properties of Stanene allows a complete and straightforward description of the phonon group velocities and phonon eigenvectors in the whole Brillouin Zone (BZ) with clear physical ingredients and a small computational effort. Phonon group velocities of a material is of great importance in predicting its thermal properties it becomes quit important in low dimension systems such as nanostructure because in low dimensional systems, understanding of propagation of phonon is of quit important as it is responsible for change in various physical properties. Here in this paper, phonon group velocities of Stanene are compared with others researchers. The theoretical predictions achieved for the phonon group velocities of Stanene are in reasonably good agreement with other researchers [19].

Acknowledgements

Appendix: Program Organizaion

In order to run the program, the user must supply the main program, depending on the use he wishes to obtain the result for group velocity on the basis of Bond Charge Model….

```python
import matplotlib.pyplot as plt
import numpy as np
import math

points = np.array([0.00, 0.05, 0.10, 0.15, 0.20, 0.25,0.30,0.35, 0.40, 0.45,0.50,0.55, 0.60, 0.65, 0.
70, 0.75, 0.80 ])

#vj = gamma
a = 4.67
vj = 0.898

def solve(fun):
  op = []
  for i in points:
    op.append(fun(i))

  return op

def vs1f(qy):
  return ((math.sqrt(3)*a)/4)*(math.sqrt(vj))*math.cos((math.sqrt(3)/4)*qy*a)

def vs2f(qy):
 return (a*(math.sqrt(9*vj)/8))*math.cos((math.sqrt(3)/4)*qy*a)

def vs3f(qx):
  return ((math.sqrt(3)*a)/2)*(math.sqrt(vj))*(math.sin((math.sqrt(3)*qx*a)/2) + math.sin(math.sqrt(3
)*qx*a))

def vs4f(qx):
  return 0

def vs5f(qx):
  return 0

def vs6f(qx):
  return (((-
a)*math.sqrt(3))/2)*(math.sqrt(11*vj))*(math.sin((math.sqrt(3)*qx*a)/2) + math.sin(math.sqrt(3)*qx*a)
)

vs1 = solve(vs1f)
vs2 = solve(vs2f)
vs3 = solve(vs3f)
vs4 = solve(vs4f)
vs5 = solve(vs5f)
vs6 = solve(vs6f)


plt.plot(points, vs1)
plt.ylabel("Phonon group velocity Vg x 10^3 (m/s)")
plt.xlabel("Wave vector (q)")
plt.plot(points, vs1, color='k', linewidth = 1,  marker = 'o')
plt.suptitle('PHONON GROUP VELOCITY OF STANENE', x=0.50, y=0.98 )
plt.legend(['TA'])
plt.show()

plt.plot(points, vs2)
plt.ylabel("Phonon group velocity Vg x 10^3 (m/s)")
plt.xlabel("Wave vector (q)")
plt.plot(points, vs2, color='k', linewidth = 1,  marker = 'o')
plt.suptitle('PHONON GROUP VELOCITY OF STANENE', x=0.50, y=0.98 )
plt.legend(['LA'])
plt.show()

plt.plot(points, vs3)
plt.ylabel("Phonon group velocity Vg x 10^3 (m/s)")
plt.xlabel("Wave vector (q)")
plt.plot(points, vs3, color='k', linewidth = 1,  marker = 'o')
plt.suptitle('PHONON GROUP VELOCITY OF STANENE', x=0.50, y=0.98 )
plt.legend(['ZA'])
plt.show()

plt.plot(points, vs4)
plt.ylabel("Phonon group velocity Vg x 10^3 (m/s)")
plt.xlabel("Wave vector (q)")
plt.plot(points, vs4, color='k', linewidth = 1,  marker = 'o')
```

```python
plt.suptitle('PHONON GROUP VELOCITY OF STANENE', x=0.50, y=0.98 )
plt.legend(['TO'])
plt.show()

plt.plot(points, vs5)
plt.ylabel("Phonon group velocity Vg x 10^3 (m/s)")
plt.xlabel("Wave vector (q)")
plt.plot(points, vs5, color='k', linewidth = 1,  marker = 'o')
plt.suptitle('PHONON GROUP VELOCITY OF STANENE', x=0.50, y=0.98 )
plt.legend(['LO'])
plt.show()

plt.plot(points, vs6)
plt.ylabel("Phonon group velocity Vg x 10^3 (m/s)")
plt.xlabel("Wave vector (q)")
plt.plot(points, vs6, color='k', linewidth = 1,  marker = 'o')
plt.suptitle('PHONON GROUP VELOCITY OF STANENE', x=0.50, y=0.98 )
plt.legend(['ZO'])
plt.show()
```

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