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Band Gap Engineering in Hexagonal Bilayer Boron Nitride: A Tight-binding Study

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Abstract. We address here the electronic band dispersion and density of states of AB staked bilayer boron nitride in a transverse applied electric field. The system is described by kinetic energy with nearest neighbor electron-hopping with hopping energy t_1 and gate potential V across for both the layers. The electron Green's functions are calculated by Zubarev's Green's function technique and electron band dispersion is found by equating the denominator of the Green's function to zero. Finally density of states is calculated from the imaginary part of the Green's function and results are interpreted by varying the different physical parameters of the system.

Keywords. Band energy dispersion, Density of states, AB- stacked bilayer BN

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1. Introduction

Two-dimensional (2D) materials have shown significant attention due to their unique structures, interesting properties, and potential applications [1]. Graphene, being one atom-thick carbon film that shows various unique properties [2]. The rise of graphene has showed the path for the discovery of other 2D materials with similar layered structure, such as hexagonal boron nitride (h-BN), transition metal dichalcogenides (TMDCs), black phosphorus (BP) [3]. Similar to graphene, these 2D materials with different chemical compositions have shown extraordinary and complementary properties, which make them promising materials for many future applications [4].

Hexagonal boron nitride (h-BN) is isomorphic to graphene in the crystalline form, which includes zero-dimensional nanocages, one dimensional nanotubes, two-dimensional atomic layers and three-dimensional bulk structure [5]. Among

the family of 2D materials, h-BN occupies a special position, being an insulator with a wide band gap (5.97 eV) iso-structural to graphene [6]. It consists of alternating boron and nitrogen atoms arranged by sp^2 bonded framework within each layer, and the bond length between B and N is 1. 44 A^0, while that in C-C in graphene is 1.42 Å [7]. The 2D h-BN has proven to be an ideal dielectric substrate of graphene for improved device quality due to its close lattice matching (~1.6%) with graphene, as well as dangling-bond free and atomically flat surface [4,5]. In the case of bilayer graphene, recent studies [8] have shown that band gap increases from 0 to 230 meV at gate potential of 3 V/nm which opens the door for bilayer graphene in electronic devices. Earlier we have reported the band dispersion of monolayer h-BN system [9]. We report here the effect of electric field on the band structures and density of states of bilayer boron nitride investigated by tight-binding approach. We present the formalism of the h-BN system in section 2, the calculation of the Green's function and the electron band structure in section 3, results and discussion in section 4 and finally conclusion in section 5.

2. A minimal tight-binding model Hamiltonian

The AB-stacked bilayer boron nitride consists of two single layers BN having each Boron atom of upper layer is placed above the corresponding Nitrogen atom of the lower layer. The single particle Hamiltonian for h-BN bilayer is given by

$$H_1 = \sum_{\alpha,k}\left[\left(E_B - (-1)^{\alpha}\frac{V}{2}\right)a^{\dagger}_{\alpha,k}a_{\alpha,k} + \left(E_N - (-1)^{\alpha}\frac{V}{2}\right)b^{\dagger}_{\alpha,k}\,b_{\alpha,k}\right] \quad (1)$$

$$H_2 = -t_1\sum_{\alpha,k}\left[\,\gamma_1(k)\,a^{\dagger}_{\alpha,k}b_{\alpha,k} + \gamma_1^{*}(k)\,b^{\dagger}_{\alpha,k}\,a_{\alpha,k}\right] \quad (2)$$

Here the Hamiltonian H_1 contains site energies E_B and E_N for boron and nitrogen atoms respectively. For symmetric band structure we have taken $E_B = 2.1\,eV, E_N = -2.1\,eV$. The term V is the applied voltage which is perpendicular to the layers with values $V = 0 - 4$ eV [10]. Here $a^{\dagger}_{\alpha,k}(a_{\alpha,k})$ and $b^{\dagger}_{\alpha,k}(\,b_{\alpha,k})$ are the creation and annihilation operators of electrons in the layers $\alpha = 1\,,2$ on the sub-lattices $A(B)$. The Hamiltonian H_2 represents for first-nearest neighbor hopping of electrons to the different sites of boron and nitrogen. As the electron hopps from boron (nitrogen) atom of the first layer to the nitrogen (boron) atom of the second layer, then interlayer Hamiltonian for BN system is given by

$$H_{\perp} = \sum_{\alpha,\beta,k} [\,\epsilon_{k,\perp} a^{\dagger}_{\alpha,k} b_{\beta,k} + \epsilon^{*}_{k,\perp}\; b^{\dagger}_{\alpha,k} a_{\beta,k} + h.c.\,] \quad \alpha,\beta = 1\,,2 \;\&\; \alpha \neq \beta \qquad (3)$$

The Hamiltonian $H_{\perp}$represents the hopping of electrons from first layer to second layer and vice-versa with interlayer hopping energy $\epsilon_{k,\perp} = t_{\perp}|\gamma_{\perp}(k)|$. Here $t_{\perp} = 0.6$ eV and $|\gamma_{\perp}(k)|$ are the perpendicular hopping integral and interlayer dispersion. The total Hamiltonian is given by $H = H_1 + H_2 + H_{\perp}$

3. Calculation of Green's functions and band dispersion h-BN bilayer system

In order to calculate the physical parameters, we calculate the four coupled electron Green's functions involving electrons of boron site atom and they are defined as

$A_{\alpha,\beta}(k,\omega) = \ll a_{\alpha,k,\sigma}\; ; a^{\dagger}_{\beta,k,\sigma} \gg_{\omega}$, where $\alpha = 1{,}2$ for two layers and $\beta = 1-4$ for four Green's function. Similarly Green's functions involving electrons of nitrogen site atoms are defined by $B_{\alpha,\beta}(k,\omega) = \ll b_{\alpha,k,\sigma}\; ; b^{\dagger}_{\beta,k,\sigma} \gg_{\omega}$. The coupled Green's functions are calculated by Zubarev's technique [11]. For first layer at A site, we find $A_{1,1}(k,\omega) = \frac{a_{22}}{2\pi|D(\omega)|}$ and for first layer at B site, we find $B_{1,1}(k,\omega) = \frac{b_{22}}{2\pi|D(\omega)|}$. Here $a_{22}\,, b_{22}$ are not given explicitly and $|D(\omega)|$ is written as $|D(\omega)| = a\omega^4 + b\omega^3 + c\omega^2 + d\omega + e$. Equating the denominator term to zero i.e. $|D(\omega)| = 0$, we can obtain the quasi-particle band dispersion energies $\omega_{\alpha,s}(k)$ which are solved numerically. Here $\mathbf{a} = 1$, $\mathbf{b} = -2(E_B + E_N)$, $\mathbf{c} = E_N^2 + E_B^2 + 4E_N E_B - \frac{V^2}{2} - 2t_1^2\gamma_1^2 - t_{\perp}^2\gamma_{\perp}^2$, $\mathbf{d} = (E_B + E_N)\left[2E_B E_N - \frac{V^2}{2} - (t_{\perp}^2\gamma_{\perp}^2 + 2t_1^2\gamma_1^2)\right]$, $\mathbf{e} = E_B^2 E_N^2 + \frac{V^4}{16} - \frac{(E_B^2+E_N^2)V^2}{4} + t_1^4\gamma_1^4 - t_1^2\gamma_1^2\left(2E_B E_N + \frac{V^2}{2}\right) - t_{\perp}^2\gamma_{\perp}^2(E_B E_N + \frac{E_B V}{2} - \frac{E_N V}{2} - \frac{V^2}{4})$. While doing all the calculations, the electron momenta appearing in the dispersion are shifted to appropriate Dirac (K) points.

4. Results and Discussion

The $|\boldsymbol{D(\omega)}| = \mathbf{0}$, which is a quartic equation, is solved numerically by taking $\mathbf{500 \times 500}$ grid points of the electron momentum in XY plane. We have obtained four electron bands $\boldsymbol{w_{11k}}, \boldsymbol{w_{12k}}, \boldsymbol{w_{21k}}$ and $\boldsymbol{w_{22k}}$ for bilayer h-BN system as shown in figure 1(a). The bands $\boldsymbol{w_{11k}}$ and $\boldsymbol{w_{12k}}$ are close to each other lying above the Fermi level and the other two bands $\boldsymbol{w_{21k}}$ and $\boldsymbol{w_{22k}}$ are close to the each other lying below the Fermi level. The minimum band gap at zero

electron momentum ($\boldsymbol{E_F}$) in the Fermi level for interlayer hopping integral $\boldsymbol{t_p = 0.6}$ is found to be $\boldsymbol{w_{12k} - w_{21k} \approx 4.2\ eV}$,which indicates that h-BN bilayer is a large band gap semiconductor which finds application in photo electron spectroscopy. The upper two bands and lower two bands merge with each other for perpendicular hopping parameter $\boldsymbol{t_p = 0}$ representing the monolayer h-BN system. The band gap in h-BN bilayer can be tuned by varying the hopping integral $\boldsymbol{t_p}$.

In figure 1(b), we show the effect of transverse electric field on electron band dispersion of bilayer h-BN. On the application of external gate potential $\boldsymbol{V = 0.6\ eV}$, the electron band $\boldsymbol{w_{11k}}$ shifts away and the band $\boldsymbol{w_{12k}}$ shifts towards the Fermi level ($\boldsymbol{E_F}$). On the other hand $\boldsymbol{w_{21k}}$ shifts upwards to approach the Fermi level. Thus the bands $\boldsymbol{w_{12k}}$ and $\boldsymbol{w_{21k}}$ are closer to the Fermi level which can describe the electron properties of the bi-layer h-BN. Here we have tuned a band gap $\Delta = \boldsymbol{w_{12k} - w_{21k} \cong 1.15\ eV}$ corresponding to $\boldsymbol{V = 3.0\ eV}$. Here the band $\boldsymbol{w_{12k}}$ lying above the Fermi level acts as conduction band and the band $\boldsymbol{w_{21k}}$ lying below the Fermi level acts as the valence band. By the application of suitable value of $\boldsymbol{V}$, one can tune band gaps of different magnitudes for application of different nano electronic devices.

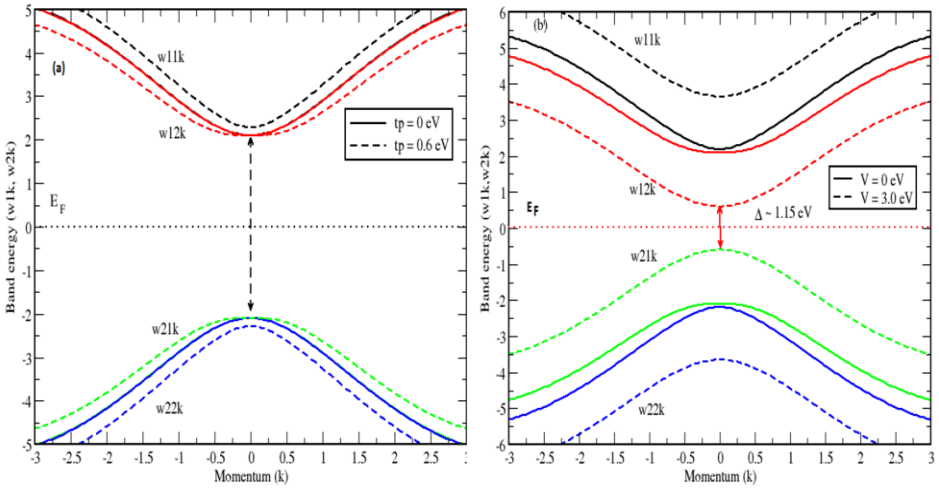

Figure 1. Plot of band energies (w1k, w2k) vs. momentum (k) for different interlayer hopping energy tp = 0 eV, 0.6 eV (see fig. a) and gate potential V = 0 eV, 3.0 eV (see fig b) in bilayer BN.

The electron density of states (DOS) calculated from the imaginary part of the electron Green's function associated with the electron at boron and nitrogen atom sites using the relation $\boldsymbol{DOS = -2\pi \sum_{k,\sigma}[A_{11}(k, \omega + i\eta) + B_{11}(k, \omega + i\eta)]}$, where $\boldsymbol{A_{11}}$, $\boldsymbol{B_{11}}$ and $\boldsymbol{\eta}$ are respectively two Green's functions and the small spectral width. In absence of transverse electric field ($\boldsymbol{V = 0}$) and interlayer hopping ($\boldsymbol{t_p = 0}$), we obtain a large gap $\boldsymbol{\Delta \cong 5.0\ eV}$ [12] separating the two peaks appearing at the van Hove singularities (not shown in figure 2). At $\boldsymbol{V = 0}$, we observe the two band structures in the DOS in presence of interlayer hopping ($\boldsymbol{t_p = 0.6\ eV}$) with the splitting of the peaks at the van-Hove singularities exhibiting the signature of the bilayer system of the h-BN and the separation between the two peaks is nearly equal to interlayer hopping energy (shown in black continuous line). Application of the transverse electric field ($\boldsymbol{V = 0.6\ eV}$), we observe that the splitting between the two peaks is enhanced. The electron density of the states of the valence band (at energy $\boldsymbol{\omega < 0}$) is reduced while the electron density of states of the conduction band is enhanced indicating that charge is transfer from valence band to conduction band. This calculated density of states represents the tunneling conductance spectra of the bilayer h-BN system [11]. On application of the transverse electric field, the band gap between conduction and valence band is reduced and hence the desired band gap of the bilayer h-BN system can be tuned for the application in nano electronic devices.

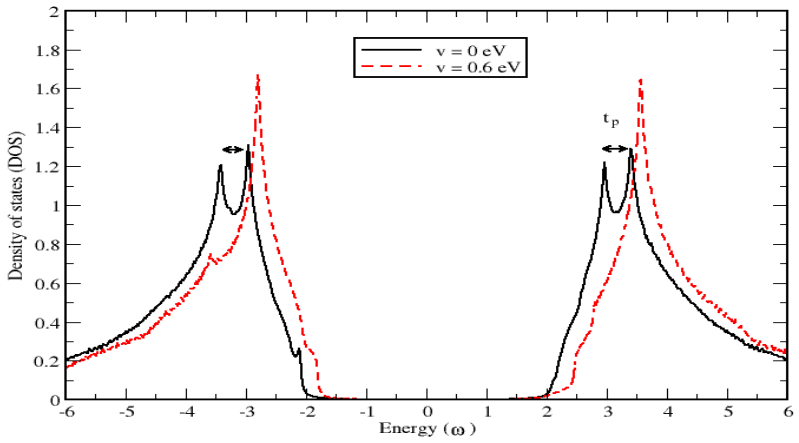

Figure 2. Plot of density of states (DOS) vs. energy (ω) for different gate potentials V = 0 eV,0.6 eV at fixed interlayer hopping energy tp = 0.6 eV in bilayer BN.

5. Conclusion

Our results suggest BN/BN layers to exhibit modulation of the band structure by electric field. The effect on electric field on BN/BN system has been characterized in earlier studies [11] and the band structure modulation described at the DFT level of theory. Our calculations on BN/BN system agree with earlier results and will be compared against the graphene/BN system to gain further insight into the modulation of band structure with the applied electric field.

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