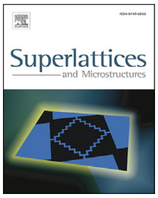
Superlattices and Microstructures 89 (2016) 204–215

Contents lists available at ScienceDirect

Superlattices and Microstructures

journal homepage: www.elsevier.com/locate/superlattices



Strain engineering the charged-impurity-limited carrier mobility in phosphorene

Yawar Mohammadi [a,*], Borhan Arghavani Nia [b]

[a] Young Researchers and Elite Club, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran
[b] Department of Physics, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran

ARTICLE INFO

Article history:
Received 13 October 2015
Accepted 29 October 2015
Available online 12 November 2015

Keywords:
Phosphorene
Tight-binding model
Band structure
Strain
Carrier mobility

ABSTRACT

We investigate, based on the tight-binding model and in the linear deformation regime, the strain dependence of the electronic band structure of phosphorene, exposed to a uniaxial strain in one of its principle directions, the normal, the armchair and the zigzag directions. We show that the electronic band structure of strained phosphorene, for the experimentally accessible carrier densities and the uniaxial strains, is well described by a strain-dependent decoupled electron–hole Hamiltonian. Then, employing the decoupled Hamiltonian, we consider the strain dependence of the charged-impurity-limited carrier mobility in phosphorene, for both types of carriers, arbitrary carrier densities and in both armchair and zigzag directions. We show that a uniaxial tensile (compressive) strain in the normal direction enhances (weakens) the anisotropy of the carrier mobility, while a uniaxial strain in the zigzag direction acts inversely. Moreover applying a uniaxial strain in the armchair direction is shown to be ineffective on the anisotropy of the carrier mobility. These will be explained based on the effects of the strains on the carrier effective masses.

1. Introduction

Since successful isolation of a single layer of graphite [1] called graphene, as the first real two-dimensional lattice structure which shows novel appealing properties [2,3], many researchers tried to synthesis or isolate new two-dimensional materials. These efforts resulted in finding other two dimensional materials such as BN [4], transition metal dichalcogenides [5], silicene [6–9] and recently phosphorene. Phosphorene is a single layer of black phosphorus, which can be isolated by mechanical exfoliation [10,11] of black phosphorus. In a single layer of black phosphorus, each phosphorus atom covalently couples to three nearest neighbours. This configuration of phosphorus atoms results in a honeycomb-like lattice structure. However, due to the sp^3 hybridization of s and p atomic orbitals, it forms a puckered surface. The electronic band structure of phosphorene has been studied using different methods such density functional theory calculations [12,13], **k.p** method [14,15] and tight-binding model [13,16,17]. These considerations show phosphorene is a direct-band-gap insulator, but with an anisotopic band structure. This novel band structure leads to many attractive properties [18–21].

Strain tuning is an effective means to tune the physical properties of two dimensional materials (for a review, see e.g. Refs. [2,22]). Puckered structure of phosphorene makes this easier, so one can tune and control its electronic and

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* Corresponding author.
E-mail address: yawar.mohammadi@gmail.com (Y. Mohammadi).

http://dx.doi.org/10.1016/j.spmi.2015.10.049
0749-6036/

mechanical properties by strain, confirmed by recent studies on the effects of uniaxial and biaxial strains in phosphorene [12,23–33]. These works examined effects of strains applied along three principle directions which preserve D_{2h} group point symmetry of phosphorene [16], its zigzag and armchair edges and the direction normal to its plane. It has been shown that a uniaxial strain in the direction normal can decrease its band gap and even leads to an insulator to metal transition [12,27,34]. Moreover, the effects of an in-plane uniaxial strains along zigzag and armchair edges [28–30] on the band gap of phosphorene has been studied. Some other researchers has studied the effects of uniaxial and biaxial strains on the band structure [30–33] and the optical properties [31] of phosphorene, confirming the capability of stain as an effective means to tune the properties of phosphorene. These works showed, when the uniaxial strain is applied along the armchair direction, the properties of phosphorene change further. But, recently, it has been shown [35] that the most effective direction to apply a strain and tune the band gap of phosphorene is an in-plane direction (not being along armchair nor along zigzag) with a direction angle about 0.268π counted from the armchair edge.

According to the high-potential capability of strains to tune the properties of phosphorene, driving an analytical relation for the Hamiltonian of strained phosphorene is very desirable, and can be used to examine the effects of the strains on the electric, optical and magnetic properties of phosphorene. In this paper, starting from the well-known 4-band tight-binging Hamiltonian of phosphorene [13,16], we obtain a strain-dependent tight-binding Hamiltonian for phosphorene. In this paper we work in the linear deformation regime and only consider uniaxial strains. To benefit from the D_{2h} group point symmetry of phosphorene and reduce the 4-band Hamiltonian to a 2-band Hamiltonian and achieve an analytical result, we restrict our consideration to the uniaxial strains applied along three principle directions of phosphorene which preserve its D_{2h} group point symmetry. Thanks to this symmetry, we can obtain analytical relations for its band energies which can be used to explore easily the effects of the uniaxial strains on properties of phosphorene. Searching for low-energy structures in strained phosphorene, we use continuum approximation and derive the corresponding Hamiltonian dominating low energy excitations. Then, by taking into account the weak interband coupling of conduction and valance bands, we project the low-energy Hamiltonian into a decoupled Hamiltonian [36–38] and show that for the experimentally accessible carrier density, the decoupled bands agree well the bands obtained from the tight-binding Hamiltonian. Motivated by this fact and the recent studies on the carrier mobility in phosphorene [10,20,37,30], then we apply our decoupled Hamiltonian to consider the strain dependence of the charged-impurity-limited carrier mobility in phosphorene. Our result shows that one can tune the amount and the anisotropy of the mobility in phosphorene, by making use of a uniaxial strain in the normal or zigzag direction.

The rest of this paper is organized as follows. In Sec. II we reproduce the known 4-band Hamiltonian of phosphorene. In Sec. III we explain how one can, in general, insert the effects of the strains in the Hamiltonian and obtain a general formalism for the strain-dependent Hamiltonian of phosphorene. Sec. IV devoted to consider the strain dependence of the charged-impurity-limited carrier mobility in phosphorene. We end the paper by summarizing our results in Sec. V.

2. Structure and tight-binding Hamiltonian of phosphorene

The lattice structure of phosphorene and the necessary lattice parameters to construct the tight-binding Hamiltonian of phosphorene, including the lattice constant, the bond angles and the transfer energies, have been introduced in Fig. 1. The unit cell of phosphorene (solid-line rectangle in Fig. 1) consists of four phosphorus atoms, two atoms in the lower layer represented by the grey circles (called A and B) and two atoms in upper layer represented by the red circles (called C and D). Hence, the tight-binding Hamiltonian of phosphorene can be written in terms of a 4×4 matrix as

$$\widehat{H}_{\mathbf{k}} = \begin{pmatrix} 0 & t_{AB}(\mathbf{k}) & t_{AC}(\mathbf{k}) & t_{AD}(\mathbf{k}) \\ t_{BA}(\mathbf{k}) & 0 & t_{BC}(\mathbf{k}) & t_{BD}(\mathbf{k}) \\ t_{CA}(\mathbf{k}) & t_{CB}(\mathbf{k}) & 0 & t_{CD}(\mathbf{k}) \\ t_{DA}(\mathbf{k}) & t_{DB}(\mathbf{k}) & t_{DC}(\mathbf{k}) & 0 \end{pmatrix}, \tag{1}$$

acting in Ref. $(\phi_A,\psi_B,\psi_C,\psi_D)^T$ with $\mathbf{k}$ being the two-dimensional momentum. Notice that $t_{BA}(\mathbf{k}) = t^*_{AB}(\mathbf{k})$. Moreover, it has been shown [13,16] that if we only retain the transfer energies up to the fifth nearest neighbours, the tight-binding approximated band structure agrees well with its density functional theory band structure. These transfer energies are [13] $t_1 = -1.220\ eV$, $t_2 = +3.665\ eV$, $t_3 = -0.205\ eV$, $t_4 = -0.105\ eV$ and $t_5 = -0.055\ eV$. So we can rewrite the Hamiltonian matrix as

$$\widehat{H}_{\mathbf{k}} = \begin{pmatrix} 0 & f_{1\mathbf{k}}+f_{3\mathbf{k}} & f_{4\mathbf{k}} & f_{2\mathbf{k}}+f_{5\mathbf{k}} \\ f^*_{1\mathbf{k}}+f^*_{3\mathbf{k}} & 0 & f_{2\mathbf{k}}+f_{5\mathbf{k}} & f_{4\mathbf{k}} \\ f^*_{4\mathbf{k}} & f^*_{2\mathbf{k}}+f^*_{5\mathbf{k}} & 0 & f_{1\mathbf{k}}+f_{3\mathbf{k}} \\ f^*_{2\mathbf{k}}+f^*_{5\mathbf{k}} & f^*_{4\mathbf{k}} & f^*_{1\mathbf{k}}+f^*_{3\mathbf{k}} & 0 \end{pmatrix}, \tag{2}$$

where the matrix elements are given by $f_{1\mathbf{k}} = 2t_1 e^{ik_x x_1}\cos(k_y y_1)$, $f_{2\mathbf{k}} = t_2 e^{ik_x x_2}$, $f_{3\mathbf{k}} = 2t_3 e^{ik_x x_3}\cos(k_y y_3)$, $f_{4\mathbf{k}} = 4t_4\cos(k_x x_4)$ $\cos(k_y y_4)$ and $f_{5\mathbf{k}} = t_5 e^{ik_x x_5}$. Here $\overrightarrow{r}_i = (x_i, y_i, z_i)$ is a vector which is drawn from A (The origin of the cartesian coordinate system) to one of the ith nearest neighbours (See Fig. 1). They are $\overrightarrow{r}_1 = (-d_1\cos\alpha, d_1\sin\alpha, 0)$, $\overrightarrow{r}_2 = (d_2\cos\theta, 0, d_2\sin\theta)$, $\overrightarrow{r}_3 = (d_1\cos\alpha + 2d_2\cos\theta, d_1\sin\alpha, 0)$, $\overrightarrow{r}_4 = (-d_1\cos\alpha - d_2\cos\theta, d_1\sin\alpha, d_2\sin\theta)$ and $\overrightarrow{r}_5 = (-2d_1\cos\alpha - d_2\cos\theta, 0, d_2\sin\theta)$ where $\cos\theta = -\cos\beta/\cos\alpha$. One can take into account the D_{2h} group point symmetry in phosphorene and project the four-band Hamiltonian into a reduced two-band Hamiltonian as [16].