Superlattices and Microstructures 83 (2015) 488–497

Contents lists available at ScienceDirect

Superlattices and Microstructures

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

Group velocity in finite graphene superlattices

M. de Dios-Leyva, R. Cuan *

Facultad de Física, Universidad de La Habana, C.P. 10400 La Habana, Cuba

ARTICLE INFO

Article history:
Received 21 March 2015
Accepted 23 March 2015
Available online 1 April 2015

Keywords:
Graphene superlattices
Band structure
Group velocity
Finite size effects

ABSTRACT

We have investigated the effects of finite crystal size on the electronic properties of infinite graphene superlattices. After deriving analytical expressions for the dispersion relation and group velocity $\boldsymbol{v}_g$ in finite N-period graphene superlattices, we demonstrated that these properties can be dramatically modified by such effects, especially those directly associated with the band structure, such as the Dirac points and the wavevector dependent minigap situated in between them. In particular, it was shown that this minigap disappears and becomes a null-gap curve. It was also shown that the properties of $\boldsymbol{v}_g$ differ substantially from those of the infinite superlattice. An interesting difference is that one of the components of $\boldsymbol{v}_g$ may attain superluminal values. Our results provide a systematical procedure for describing and understanding the electronic transport and optical characteristics of any finite N-period graphene superlattices, such as the density of states, conductivity and absorption coefficient.

1. Introduction

The transport of charge carriers through periodic one-dimensional (1D) superlattices (SLs) in monolayer graphene, has been the subject of considerable interest in the last years [1–8]. This interest is motivated by the unusual transport properties discovered in these structures, and by potential applications in a wide range of electronic devices. A quantity of fundamental importance in these studies is the group velocity, defined as

---

* Corresponding author.
E-mail address: rcuan@fisica.uh.cu (R. Cuan).

http://dx.doi.org/10.1016/j.spmi.2015.03.046

$$\boldsymbol{v}_g = \frac{1}{\hbar}\nabla_{\boldsymbol{k}}E(\boldsymbol{k}), \tag{1}$$

where $\boldsymbol{k}$ is the wavevector and $E(\boldsymbol{k})$ represents the SL dispersion relation, which exhibits properties that are in general different from those of the original graphene. For instance, the band structure of a graphene SL exhibits additional Dirac points or cones [3,9–12], which clearly departs from the observed in the pristine graphene. As is well known, the presence of these cones can significantly affect the properties of physical quantities closely related to the transport of charge carrier, such as the density of states [3,10], conductivity [3,4,8], Landau levels [13,14] and group velocity [6,9,13]. Actually, while the group velocity around the Dirac point of the original graphene shows an isotropic behavior, in the SL it may be highly anisotropic, leading to the possibility of collimation [15] of electrons, and to significant modifications of the conductivity. Thus, the group velocity plays a prominent role in the description and understanding of the electronic transport in graphene SL.

Now, in accordance with Eq. (1), when studying theoretically the properties of $\boldsymbol{v}_g$, it is necessary to know the dispersion relation $E(\boldsymbol{k})$ of the graphene SL, which up to now has been essentially addressed for infinite periodic SLs. These are media with translational symmetry, thus $E(\boldsymbol{k})$ — and consequently $\boldsymbol{v}_g$ — are obtained by applying the Bloch–Floquet theorem. It is then clear that when this symmetry is broken, as occur when effects associated with disorder or finite crystal size are considered, this theorem is no longer valid and the properties of the group velocity may be substantially modified.

In this work, we will present a detailed theoretical study of the effects of finite crystal size on the properties of the dispersion relation and group velocity of chiral electrons in graphene SLs. To carry out this study we use a finite N-period SL, modeling the corresponding 1D potential $V(x)$ via the Kronig–Penney model. This approach allows us to obtain analytical expressions for the band structure (Section 2) and group velocity (Section 3), which were then used to demonstrate the consequences of these effects on the infinite SL properties, including those associated with the Dirac cones, density of states, conductivity and absorption coefficient.

2. Dispersion relations

To derive the mentioned expression for the group velocity, it is necessary to obtain the equation determining the dispersion relation of the N-period SL which can be defined in terms of the complex transmission coefficient [16,17]. This require then to study the process of scattering shown schematically in Fig. 1. The scattering region corresponds to a $[BABA\ldots BA]$ finite N-period SL, which we suppose localized between the $x = 0$ and $x = L$ lines, sandwiched between two semi-infinite layers A of graphene. We choose y to represent the lateral direction. The structure has a lattice constant $d = a + b$, where a and b are the widths of layers A (well) and B (barrier), respectively. The potential along the SL is taking as $-V_0/2$ at the emitter ($x \leqslant 0$) and collector ($x \geqslant L$) terminals, and also in the wells A, whereas $V(x) = V_0/2$ in the barriers B.

Limiting ourselves to the case of SL electronic states in the vicinity of the K point in the Brillouin zone (BZ), the spatial part of the stationary scattering state of an electron may be described by a two-component spinorial wave function $\boldsymbol{\Psi}(\boldsymbol{r})$, satisfying the Dirac-like equation

$$\hat{\boldsymbol{H}}\boldsymbol{\Psi}(\boldsymbol{r}) = \{v_F\boldsymbol{\sigma}\cdot\hat{\boldsymbol{p}} + V(x)\boldsymbol{I}\}\boldsymbol{\Psi}(\boldsymbol{r}) = E\boldsymbol{\Psi}(\boldsymbol{r}), \tag{2}$$

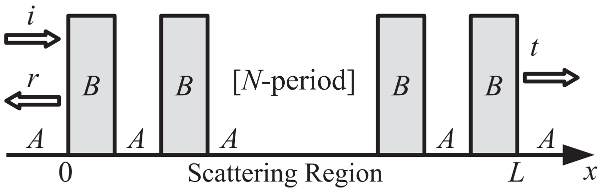

Fig. 1. Schematic of the process of scattering by a finite N-period SL, composed of alternating layers of barriers B and wells A of graphene, localized between the $x = 0$ and $x = L$ lines and sandwiched between two semi-infinite layers A of original graphene. Arrows indicate the incident, reflected and transmitted waves.