Theoretical Study of Graphene Nanoribbon Photo-Detectors

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Graphite-related materials such as carbon nanotubes (CNTs) and graphene have been extensively studied in recent years due to their exceptional electronic, opto-electronic, and mechanical properties. However, the limited control over the chirality and diameter of CNTs and thus of the associated electronic bandgap remains a major technological problem. Recently, graphene sheets have been patterned into narrow nanoribbons [1]. The electronic properties of GNRs exhibit a dependence on the ribbon direction and width. The electronic band structure of GNRs depends on the nature of their edges: zigzag or armchair[2, 3].

In Fig. 1-a, a honeycomb lattice having armchair edges along the x direction is shown. In comparison with CNTs, there are key potential advantages in designing and constructing device architectures based on GNRs [4]. The direct bandgap and the tunability of the relatively narrow bandgap with the ribbon’s width enables them as suitable candidates for opto-electronic devices, especially for infra-red applications. The non-equilibrium Green’s function (NEGF) formalism is used in this work to perform a comprehensive study of photo detectors based on graphene nanoribbons. The device response is studied for a wide range of photon energies. The energy conversion efficiency as a function of the incident photon energy, ribbon’s width, and orientation is evaluated.

The atomistic real space tight-binding approach for the description of the electronic bandstructure has been used [5]. For device simulation the Hamiltonian of electron-photon interaction in real space has been employed [6]:

$$\hat{H}_{e-ph} = \sum_{l,m} M_{l,m} \left( b e^{-i\omega t} + b^\dagger e^{i\omega t} \right) \hat{a}_l^\dagger \hat{a}_m, \quad M_{l,m} = (z_m - z_l) \frac{ie}{\hbar} \sqrt{\frac{\hbar\omega}{2N\omega c}} (l|\hat{H}_0|m)$$

Using this type of Hamiltonian the effect of electron-photon interaction is considered by adding the respective self-energy, $\Sigma_{l,m}(E) = \sum_{p,q} M_{l,p} M_{q,m} \times NG_{p,q}(E - \hbar\omega)$, into the kinetic equations [6, 7]. The incident light is assumed to be monochromatic, with polarization along the x direction. Fig. 1-b shows the density for the first three subbands of an (12, 0) armchair GNR. Van Hove singularities in the density of states result in large photon-assisted transitions from the valence to the conduction direction. The electronic band structure of GNRs depends on the nature of their edges: zigzag or armchair[2, 3].

To investigate GNR photodetectors we study the quantum efficiency which is defined as $\alpha = (I_{ph}/q)/(P_{op}/\hbar\omega)$, where $I_{ph}$ is the photo current and $P_{op}$ is the incident optical power. This quantity corresponds in fact to the energy conversion efficiency of a photodetector. Fig. 2 compares the quantum efficiency of a 6-armchair and 6-zigzag GNR device as a function of the incident photon energy. The efficiency is maximized, when the photon energy matches the bandgap of the GNR. The maximum quantum efficiency ranges from 9% to 11% and is fairly independent of the bandgap [7]. An experimental and a theoretical study of CNT based photodetectors has estimated a quantum efficiency in the $10$–$20\%$ range [7, 9]. Due to periodic boundary conditions, the subbands of CNTs are doubly degenerate. However, in GNRs this symmetry is removed and subbands are no longer degenerate. As a result the photo-current in GNRs is roughly half of that of their CNT counterparts. It is, therefore, reasonable to expect a maximum quantum efficiency of $10\%$ in GNR devices. As the width of the GNR increases the band-gap decreases and transitions at lower energies will be possible (infra-red range). Fig. 3 compares the calculated quantum efficiency for a 12-armchair and a 18-armchair GNR. The results indicate that the quantum efficiency decreases as the width increases. This behavior can be well understood by considering the fact that as the width increases the number of subbands and respective allowed transitions increases. However, the maximum current capacity of each subband remains nearly unchanged. In fact due to the confinement along the transverse direction the conductance of each subband is quantized with a maximum value of $G = 2q/h$. As the width of the ribbon increases the incident optical power increases, whereas the photo-current is not scaled, resulting in the reduction of the quantum efficiency. Another figure of merit of interest for photodetectors is the photo-responsivity given by $I_{ph}/P_{op}$. Our calculations give an upper limit for the responsivity of 0.15 A/W for photon energies near the GNR band gap, which is nearly half of that of CNTs [7].

In summary, we present a study of GNR-based photo-detectors employing the NEGF method. Due to the lack of band-degeneracy, the photo-current in GNR devices is roughly half of that of their CNT counterparts. Although CNT photodetectors show better performance, the fabrication of GNRs is more compatible with current semiconductor technologies, which renders them well suitable for future opto-electronic applications.

REFERENCES

Figure 1: a) The sketch of an armchair GNR based photodetector. The incident light is assumed to be polarized along the $x$ direction. b) The density of states of an $(12, 0)$ armchair GNR. Some of the most important transitions are marked: $E_{ij}$ denotes a transition from the $i^{th}$ valence to the $j^{th}$ conduction band.

Figure 2: a) The quantum efficiency of a 6-armchair GNR as a function of the incident photon (solid black). b) The quantum efficiency of a 6-zigzag GNR. For a better comparison the normalized quantity $\text{JDOS}(\omega)/\omega$, where the joint density of states is defined as $\text{JDOS}(\omega) = \sum_{k,v,c} \delta(E_c(k) - E_v(k) - \hbar\omega)$, is also shown (blue dashed). Although a large density of states is available, only few transitions are allowed.

Figure 3: The quantum efficiency of a a) 12-armchair b) 18-armchair GNR as a function of the incident photon (solid black). The normalized quantity $\text{JDOS}(\omega)/\omega$ is also shown (dashed blue).