A NUMERICAL STUDY OF GRAPHENE NANO-RIBBON BASED RESONANT TUNNELING DIODES

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A numerical study of graphene nano-ribbon (GNR) based resonant tunneling diodes (RTD) is presented. The non-equilibrium Green's function formalism has been employed to investigate the current-voltage characteristics of a GNR based RTD.

The many desirable material properties of the novel graphene films, including ultra-high mobility, high saturation velocity, high current carrying capability, excellent thermal conductivity, ultra-thin geometry, and the feature to integrate with traditional CMOS processes, offer the potential for graphene-based electronics. Since the bandgap of semiconducting GNRs is inversely proportional to their width, hetero-junctions using GNRs of different widths can be envisioned. A rich variety of bandgaps in GNRs has been discussed in [1]. They are either metals or semiconductors depending on their edge shape and width. Two nano-ribbon segments with different atomic and electronic structures can be seamlessly fused together to create intermolecular metal-metal, metal-semiconductor, or semiconductor-semiconductor junctions. Moreover, periodically repeating hetero-junctions of different widths can form superlattices [2]. Since nano-ribbons with a width less than 10 nm with uniform and patterned edges have been produced [3], present results related with graphene based nano-ribbons and their hetero-junctions of diverse geometry can, in fact, be a candidate for a class of nano-devices with a richness of novel properties.

Ref [4] has suggested a double barrier resonant tunneling device by employing several segments of armchair GNRs with different widths. The density functional theory (DFT) to study such devices was employed; however, the DFT method is suitable only for closed quantum systems in equilibrium. We employed the non-equilibrium Green's function (NEGF) formalism which is a rigorous technique for investigating open quantum systems in a non-equilibrium condition [5].

In graphene three σ bonds hybridize in an sp^2 configuration, whereas the other $2p_z$ orbital, which is perpendicular to the graphene layer, forms π covalent bonds [6]. The π energy bands are predominantly determining the solid state properties of graphene. We use a nearest-neighbor tight-binding π-bond model. Each atom in an sp^2-coordinated graphene has three nearest neighbors, located $a_{cc} = 1.42$ °A away. The band-structure consists of π-orbitals only, with the hopping parameter $t \approx -2.7$ eV. Figure 1 shows the analyzed structure. Potential barriers appear in the regions where the width of the GNR is reduced and confined states form in the quantum well. As shown in Fig. 2, when the Fermi level in the left contact matches with any of these states, a peak in the current-voltage characteristics appears. Our results show that the specific device operates with a resonant tunneling double barrier with resonances determined by the quantum well states. The device characteristics can therefore be constructively engineered by proper design of the layer structure.

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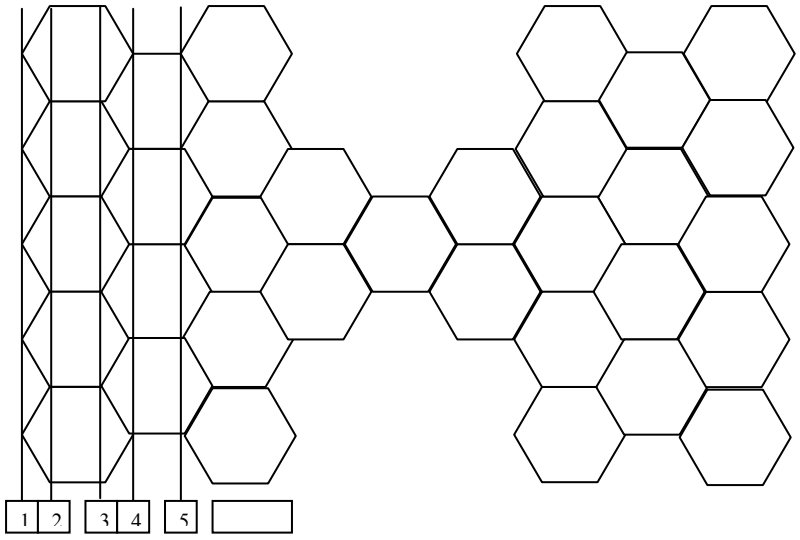

Figure1: Layer layout of the simulated device. This figure shows half of the device.

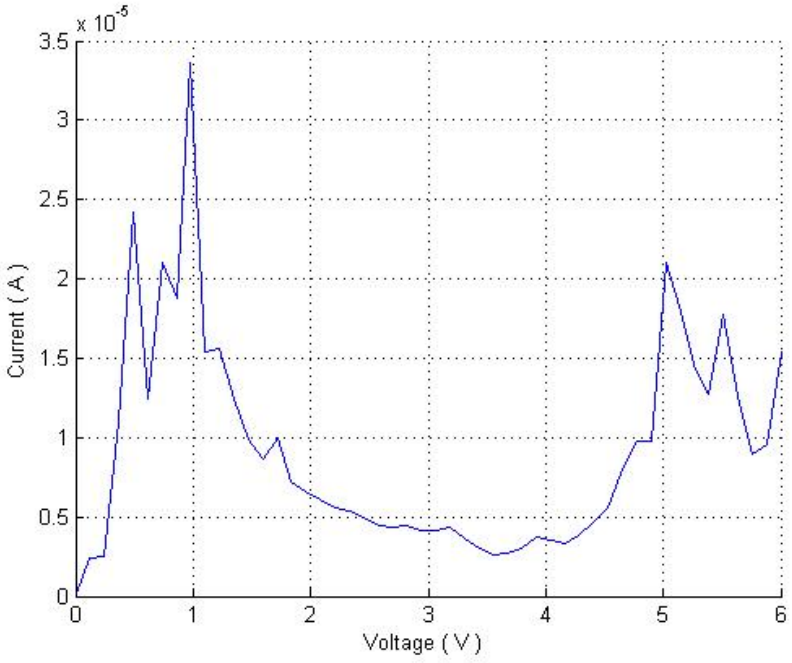

Figure 2: Current-voltage characteristics of the simulated device.