Abstract—We show that recently fabricated Chevron-type graphene nanoribbons act as a monolithic superlattice structure. This is enabled by the large periodic unit cells with regions of different effective bandgaps in these nanoribbons, resulting in minibands and gaps in the density of states above the conduction band edge. Quantum transport calculations based on non-equilibrium Green's function formalism reveal that a negative differential resistance (NDR) is expected to manifest in these nanoribbons. Due to the relatively low density of states, such NDR behavior can also be modulated with a gate electric field. We show that a sub-thermal subthreshold swing ($kT/q$) can potentially be obtained in a three-terminal configuration, even in the presence of optical phonon scattering.

Index Terms—Graphene nanoribbons, steep-slope switch, negative differential resistance, quantum transport.

Unlike an Esaki diode, superlattices could provide negative differential resistance without the need of tunneling [1]. Nonetheless, significant difficulty in synthesizing atomically precise, epitaxial heterostructures has made it very challenging to realize such superlattice structures [2]–[8]. In recent years, much work has been done on superlattices involving graphene nanoribbon (GNR) and carbon nanotube (CNT) heterostructure and superlattices and also III-V nanowire heterostructure within the context of steep subthreshold tunnel transistors (TFET) [9]–[18]. However, the difficulty in artificially synthesizing these heterostructures remains. Here, we show that the recently synthesized chevron nanoribbons [19] (CGNR) provide a natural, monolithic material system where superlattice-like narrow-width energy bands and negative differential resistance (NDR) can be achieved. Importantly, the edge roughness that plagues device performance in conventional GNRs [20], [21] can be avoided as it was experimentally demonstrated that such chevron GNRs can be synthesized with atomistically pristine edge states [19], [22]–[24].

Fig. 1(a) shows both the structure of the 6-9 CGNR originally fabricated by Cai et al. and the band structure calculated with a $p_z$ orbital-based tight-binding method [19]. A key feature of the band structure is the presence of minibands with regions of forbidden energy above the conduction band edge, such as those seen in superlattices of III-V semiconductors. When we look at the CGNR in Fig. 1(a), we see that its narrowest segment is 6 carbon atoms across, and its widest segment is 9 carbon atoms across, with both segments having armchair-type edges. Using a $p_z$-basis set (GW [25]), the bandgap, $E_g$, of a 6-AGNR is 1.33 eV (2.7 eV) and the bandgap of a 9-AGNR is 0.95 eV (2.0 eV). However, given the very short length scale over which the width changes in our structure (≈1 nm), one would not expect the system to behave as though the local effective potential oscillates between the bulk values of $E_g$ for the isolated AGNRs. In fact, our chevron structure has an overall bandgap of 1.59 eV.
to those used by Koswatta et al. for phonon coupling constants, we use approximate values similar in [29]–[33]. Because we lack an exact value for the electron taken into account with the according to the method described three dimensions. Acoustic and optical phonon scattering are solved self-consistently with the nonlinear Poisson equation in parameters are shown in TABLE I.

This value is consistent with the 1.62 eV bandgap from LDA DFT calculations, but significantly smaller than the 3.74 eV value from calculations incorporating the GW correction [26]. Both LDA and GW calculations show the presence of minibands and gaps above the conduction band edge [26]. We also calculated the CGNR band structure with the pd tight-binding model of Boykin et al. [27] and find good agreement with the results obtained from px basis set.

Within this model, the bandgap was 1.50 eV and the width of the first miniband for the conduction band was 71 meV, lower than the 272 meV value for the px Hamiltonian. However the width of the first miniband in the valence band was 314 meV, consistent with the bandwidth in px model, which is symmetric for conduction and valence bands. The gap between the first and second of minibands was 187 meV, which is symmetric for conduction and valence bands. The local density of states for the CGNR MOSFET is shown in Fig. 2 for several biasing conditions. Fig. 2b shows peak current case when a large enough drain bias has been applied to generate enough splitting between the source and drain Fermi levels to allow significant current to flow, but not a high enough bias to move the first miniband outside of the current conduction window. Fig. 3, nearly all conduction occurs solely through phonon-assisted tunneling. For higher bias as in Fig. 2c, intraband conduction from the first miniband is completely cut off, though a significant current continues to flow because of optical phonon scattering. As the drain bias is further increased, current can only flow due to band-to-band tunneling from the first miniband to the second miniband becomes possible, and current increases again. The second feature of the device is that the superlattice gap at the drain filters out higher energy electrons from the first miniband at the source when a source-drain bias is applied. This cuts off the higher energy portion of the Fermi function at the source, resulting in energy filtering as in a TFET. Transport in this device, however, is entirely intraband like a MOSFET, whereas a TFET relies on band-to-band tunneling. This could possibly allow higher ON current than a TFET.

The CGNR used in our simulation has a width of 1.9 nm. The simulation domain is approximately 70 nm long, and the gate has a length of 15 nm. The source and drain are doped with N = 1.0 × 10^{13} cm\(^{-2}\) donors. An effective oxide thickness of 1.0 nm is used for both the top and bottom gates. The gate contacts are extended 30 nm perpendicular to the channel to capture fringing gate fields. While our simulation uses an effective doping density to align the source and drain Fermi levels to the CGNR conduction band, this could be achieved in an experiment through electrostatics alone. The parameters for the simulation are listed in Table I.

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Figure 3 shows the energy-resolved current spectrum in the OFF state at $V_{gs} = 0.55 \text{ V}, V_{ds} = 0.10 \text{ V}$ (the same bias point as Fig. 2a). In the OFF-state, subthreshold leakage current is suppressed because of the lack of states at the drain at the energy of the top of the barrier. However, optical phonon scattering permits some carriers to be scattered down into the first miniband at the drain. Nevertheless, the steep-slope behavior is preserved, despite being deteriorated relative to 6 mV/decade subthreshold swing observed in ballistic calculations. Previously, Yoon and Salahuddin [33] studied the effects of phonon-assisted band-to-band tunneling in AGNR tunnel transistors. That work concluded that while subthreshold swing in those devices was degraded by electron-phonon scattering, it was still possible to achieve a subthreshold swing of 34 mV/decade, far below the Boltzmann limit, consistent with the degradation in performance we see in our device when the effects of the electron-phonon interaction are considered.

Previous work on III-V MOSFETs with a superlattice source filter by Lam et al. [34] found that it should be possible to achieve $I_{ON} = 0.81 \text{ mA } \mu \text{m}^{-1}$ with $SS = 20.9 \text{ mV/decade}$ at $V_{ds} = 0.6 \text{ V}$, though this calculation did not take into account phonon scattering. Assuming a device with multiple ribbons in parallel with a pitch of 5 nm, our device achieves $I_{ON} = 0.017 \text{ mA } \mu \text{m}^{-1}$. While this value is much smaller, our device operates $V_{ds} = 0.1 \text{ V}$. Because of the NDR effect, higher drain biases unfortunately result in lower current.

In summary, we have shown that CGNR devices can exhibit both steep-slope subthreshold behavior and negative differential resistance. Both properties are the result of the superlattice-like electronic structure of the ribbon. CGNR SLFETs could be promising for a number of applications ranging from low-power logic transistors to high speed oscillators. A major obstacle to building a real device is making contacts with appropriate Schottky barrier heights to be able to match the band alignment conditions achieved in this work through doping. The performance of a real device could also be impacted by edge roughness, which we have not considered here, though the ability to synthesize ribbons with virtually no defects may minimize this effect. Additional optimization is also likely necessary to make a functioning device. DFT+GW calculations predict a much higher bandgap for the CGNR in vacuum than the tight-binding model used in this work. While surface screening may reduce the bandgap, a wider ribbon with a narrower bandgap may be required. Co-optimization of the bandgap with the bandwidths of the minibands and the gaps between minibands is also a necessary topic for future work.

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REFERENCES


