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Combined effect of edge roughness and phonon scattering on the electronic properties of ultra scaled graphene nano-ribbons

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ABSTRACT

The effect of optical and acoustic phonon-scattering in the presence of line-edge-roughness (LER) on the electronic properties of ultra-scaled armchair graphene nano-ribbons (AGNRs) is investigated. Non-equilibrium Green's function formalism (NEGF) is employed using a Hamiltonian formed from tight bonding model with consideration of first and third nearest neighbors. The combined effect of phonons and line edge roughness on the transmission, transport gap, and conductance are studied for different roughness strengths and AGNR lengths. Results show edge roughness slightly reduces the onset of optical phonon emission, acoustic phonons reduce off-state conductance and optical phonons reduce on-state conductance. In both cases, the degree and behavior of reduction is totally dependent on the intensity of edge roughness. Also, in the longer AGNRs with high edge roughness intensity, phonons increase the transport gap.

1. Introduction

Ever since graphene was first successfully separated from graphite flakes in 2004 [1] and its unique properties such as high mobility [2] and tunable band-gap with width [3] were discovered, great

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interest has been shown in investigating and studying graphene in scientific circles. Large strips of graphene display metallic properties and must be cut into narrow strips to create semiconducting properties and a bandgap [4]. Among these strips, Armchair Graphene Nanoribbons (AGNRs) are better suited for field effect transistor (FET) channels. Studies on the electronic transport properties of AGNRs have shown that line-edge-roughness (LER) plays a dominant role in scattering [5,6]. LER is caused by removing or adding atoms at the boundaries of the AGNR. In addition to LER, optical and acoustic phonon scattering further deteriorate the electronic properties of perfect AGNRs [7–9]. In a previous study, the combined effects of phonons and edge roughness have been studied on a small scale in GNR tunneling field effect transistors [10] that focused on ten samples with 70 nm long channels. Since graphene is a fairly promising candidate in achieving the goal of the 12 nm and below technology node [11,12] as set out by the International Technology Roadmap for Semiconductors (ITRS), AGNRs with sub 10 nm lengths are chosen to demonstrate the combined effect of phonons and LER on the electronic properties of AGNRs. This article will focus on the effects of AGNR length and roughness intensity combined with phonon scattering on different electrical properties of these AGNRs.

2. Materials and methods

2.1. Tight binding model

To study the properties of AGNRs, originally a first nearest neighbor tight binding model was employed. The results showed that one third of all ribbons must show metallic properties, but these theoretical results were inconsistent with experimental data that showed all AGNRs were semiconductors. Subsequently, results obtained from third-nearest-neighbor (TNN) tight-binding models showed that TNN models more accurately presented the properties of AGNRs [13]. The second nearest neighbor is usually omitted because it does not influence carrier transport [9] and only complicates the computation process. The hopping parameters between first and third nearest neighbors are mostly selected as $t_{i,j} = -2.7$ eV and $t_{i,m} = -0.3$ eV respectively [14]. The subscript i encompasses all grid points while j and m are restricted to first and third neighbors of i.

2.2. Line edge roughness

In the current study LER is modeled stochastically by using an exponential autocorrelation function [15]:

$$R(X) = \Delta W^2 \exp\left(-\frac{|x|}{\Delta L}\right), \; x = n\Delta x \tag{1}$$

ΔW denotes the root mean square of the fluctuation amplitude, ΔL shows the roughness correlation length, and Δx is the sampling interval which is equal to half the lattice constant ($a_{cc}/2$). To create LER in real space, first the power spectrum of the autocorrelation function is obtained by calculating its Fourier transform then a random phase is applied to the power spectrum. The inverse Fourier transform gives roughness in real space [16].

2.3. NEGF formalism and phonon scattering

Simulations are performed by using the standard Green's Function method [17,21]. The surface Green Functions are calculated using the Sancho-Rubio method [19]. To take into account electron–phonon scattering, the Born self-consistent procedure [9,20–22] is used. Transmission for elastic scattering is obtained by using the standard Laundauer-Buttiker formalism and for inelastic scattering an effective transmission function demonstrated by Datta can be used [18].

3. Numerical results

To evaluate the combined role of phonons and line edge roughness on the electrical properties of ultra-scaled AGNRs a ribbon with a width of 1 nm is utilized. The device is simulated for lengths