Disorder-induced variability of transport properties of sub-5 nm-wide graphene nanoribbons

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Abstract
Transport properties of sub-5 nm-wide graphene nanoribbons (GNRs) are investigated by using atomistic non-equilibrium Green’s function (NEGF) simulations and semiclassical mobility simulations of large ensembles of randomly generated nanoribbons. Realistic GNRs with dimensions targeting the 12 nm CMOS node are investigated by accounting for edge defects, vacancies and potential fluctuations. Effects of disorder on transmission, transport gap, mean free path, density of states and acoustic phonon limited carrier mobility are explored for various disorder strengths and GNR widths in the 1–5 nm range. We report the high variability of GNR transport properties that could be a strong limiter for potential nanoelectronics applications of GNRs.

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1. Introduction

Graphene is a promising material for future nanoelectronic devices because of its high carrier mobility that offers a possibility of ballistic transport over large distances at room temperature [1]. Furthermore, graphene is compatible with the planar CMOS technology due to its two-dimensional structure. The problem of large OFF state current and low ON–OFF current ratios in graphene, which is caused by the zero bandgap, can be resolved by patterning graphene into graphene nanoribbons (GNRs) [2,3]. In contrast to graphene, GNRs have parabolic bands and a bandgap, which is a consequence of quantum confinement [4,5]. However, massive carriers decrease the mobility in GNRs in comparison with the large-area graphene [6,7], which introduces a trade-off between the acceptable bandgap and satisfactory mobility.

In this paper, we calculate the transport properties of realistic GNRs that include disorder such as edge defects or vacancies, which are a consequence of fabrication processes, and potential fluctuations that are caused e.g. by charged impurities in the substrate. The effects of lattice defects and potential disorder have been studied previously in graphene [8,9] and to a certain extent in GNRs, but mostly for larger nanoribbons [10], specific disorder cases [11,12] and for small ensembles of devices [13,14]. In contrast to the previous reports, we study large ensembles of GNRs with different widths and various disorder strengths, and we focus on GNR dimensions that target the 12 nm CMOS node [15], i.e. length of ~10 nm and widths under 5 nm for acceptable bandgaps [5,16].

The goal of our study is to explore the transport properties of extremely narrow realistic GNRs by using atomistic quantum transport and semiclassical mobility simulations. This paper reports the relative influence of three main disorders (edge defects, vacancies and potential fluctuations) on transmission, transport gap ($E_{Tg}$) and density of states (DOS), for various disorder strengths. Since a statistical approach is used, we examine the transport properties that are averaged over an ensemble of randomly generated GNRs. In addition, we study the variability of the transmission, $E_{Tg}$ and DOS. The possibility of ballistic transport due to ultra-short channel length is explored in disordered GNRs by calculating the mean free path (MFP). Finally, using the findings from the quantum transport simulations, an analytical model for the DOS of disordered GNRs is proposed and employed to investigate the features of mobility limited by acoustic phonons, i.e. its variability and the behavior with the downscaling of the GNR width.

2. Atomistic NEGF simulations of GNRs

The simulated devices are semiconducting armchair GNRs that belong to the same $3k + 1$ group for consistency. Nanoribbon length ($L$) is 10.1 nm, while the width ($W$) ranges from 1.10 nm to 4.80 nm. We use a tight-binding Hamiltonian, in which each carbon atom is represented with a single $p_z$ orbital, of the following form
where $\varepsilon_i$ is the on-site energy and $c_i^\dagger$ ($c_i$) is the creation (annihilation) operator. The Hamiltonian accounts for the nearest, second-nearest, and third-nearest neighbor interaction with $t_1$, $t_2$ and $t_3$ being the respective hopping parameters [17]. For carbon–carbon bonds at the edges of the GNR we use a modified hopping parameter $t'_i$ in order to account for the edge-bond relaxation effect that increases the bandgap [16].

The non-equilibrium Green’s function (NEGF) approach [18–20] is employed to calculate the transmission, density of states, and atomically-resolved local DOS (LDOS). The Green’s function of the device is found using

$$G_d = (\omega I + H - \Sigma_1 - \Sigma_2)^{-1},$$

where $H$ is the device Hamiltonian obtained from (1), and $\Sigma_1, 2$ are the contact self-energies that account for the coupling between the device and the contacts. The DOS and LDOS are calculated from the diagonal elements of the spectral function matrix $A(E) = (G_d - E)$.

The transmission function between the ideal semi-infinite contacts 1 and 2 (i.e. source and drain) is found using

$$T_{12}(E) = \text{Trace}(\Gamma_1 G_d \Gamma_2 G_d^\dagger),$$

where $\Gamma_{1,2}$ are the contact broadening functions.

Lattice defects are implemented by random removal of single carbon atoms from the lattice in the given percentage, either from the edges (edge defects, $P_{\text{ED}}$) or from the bulk (vacancies, $P_v$) of the GNR, as illustrated in Fig. 1a. Orbitals of the missing atoms are removed from the total Hamiltonian by setting the respective hopping parameters to zero. In this work, we neglect the reconstruction and relaxation of the defected lattice. Potential fluctuations are randomly generated as positive and negative Gaussian potential profiles with an amplitude $\delta V$, illustrated in Fig. 1b, as we assume that they are caused by the charged impurities in the substrate. The fluctuations are implemented in the Hamiltonian as local shifts in the on-site energy [21,22].

3. Results and discussion

3.1. Influence of disorder on the transmission

The effects of different disorder strengths on the transmission of 2.58 nm-wide GNR are presented in Fig. 2a–c for edge defects, vacancies and potential fluctuations, respectively. The transmission curves are averaged over $N = 100$ randomly generated GNRs for each disorder case in Fig. 2. Edge defects suppress the transmission over the whole energy range with a stronger effect at lower energies. However, the decrease in transmission saturates for higher $P_{\text{ED}}$ values. Namely, if we extract the transport gap at $T_{12} = 0.01$ it is difficult to establish a clear trend in gap behavior as $P_{\text{ED}}$ increases. From the results in Fig. 2a we find that $E_T$ values are comparable despite a large difference of edge defect densities. The observed behavior of the transmission is in qualitative and quantitative contrast to that found in narrower edge-defected GNRs, i.e. sub-2 nm-wide GNRs exhibit strong transmission suppression as $P_{\text{ED}}$ increases and the enhancement of the transport gap is clearly observed [22]. However, for the GNR with $W = 2.58$ nm the averaged transmission is enhanced in the low-energy region, which is due to a small difference in $E_T$ being the respective hopping parameters.

The introduction of vacancies into the GNR causes a strong suppression of the transmission over the whole energy range, as shown in Fig. 2b. The averaged transmission curves of GNRs with vacancies reveal that $E_T$ increases monotonically as $P_v$ increases, in contrast to the 2.58 nm-wide GNR with edge defects. In the case of high vacancy density, we note the occurrence of transmission peaks in the averaged transmission at certain energies in sub-1 eV energy range. As demonstrated in Fig. 2c, potential fluctuations have a modest influence on the transmission and a negligible effect on the transport gap within the quantum transport approach, even for the amplitude $\delta V$ of 500 mV. We find that the device is immune to potential disorder since the transmission is negligibly reduced for realistic amplitudes $\delta V < 100$ mV. Unlike the case of edge defects, the properties of the 2.58 nm-wide GNR with vacancies and potential fluctuations qualitatively agree with those in sub-2 nm-wide nanoribbons [22].

In order to clarify the $E_T$ behavior in edge-defected GNRs, where a saturation behavior is observed with increasing $P_{\text{ED}}$, we investigate the correlation between the transmission and LDOS. An advantage of using atomistic NEGF simulations is that we can investigate LDOS at any given energy and study the effects of localization. Fig. 3a shows a transmission function of a single randomly generated GNR with $P_{\text{ED}} = 50$% with letters $b,c,d$ and $e$ marking certain transmission maxima and minima. Atomically-resolved LDOS at energies of 0.22, 0.30, 0.36 and 0.82 eV are shown in Fig. 3b–e, respectively, with the energies corresponding to the energies where the transmission maxima and minima occur. An extended state is shown in Fig. 3e, whereas localized states are observed in Fig. 3b–d. According to the mobility-edge theory [10,23–25], localized states do not contribute to conduction, while the opposite is true for the extended states. We note that the cases

![Fig. 1.](image-url)
in Fig. 3b, c and e correspond to local transmission maxima, whereas the case in Fig. 3d corresponds to the local minimum of the transmission curve in Fig. 3a. Therefore, states at energies of 0.22 eV and 0.30 eV exhibit high transmission despite being localized. In other words, we find that the transmission function can exhibit a peak while at the same time the LDOS can indicate strong localization. In contrast to the localized state at \( E = 0.36 \) eV (Fig. 3d), localized states at 0.22 eV (Fig. 3b) and 0.30 eV (Fig. 3c) exhibit larger quantum transmission due to the more favorable distribution of the localized states. Namely, in Fig. 3d localized states are separated by almost the whole GNR length, which effectively shuts off the transmission. Since the grouping and separation between localized states seems to be the most important factor determining the transmission value, it is likely that the effect of enhanced transmission is related to variable range hopping (VRH) [26–28]. Within VRH, the quantum transmission depends on the spatial and energy separation between the localized states and is proportional to

\[ T_{12} \propto \exp \left( -2R/\bar{z} \right) \exp \left( -\Delta E/k_B T \right), \]

where \( R \) is the average distance between localized states, \( \bar{z} \) is the localization length, and \( \Delta E \) is the energy difference between states. To obtain the expression for the ratio between transmission at points \( b \) and \( d \) in Fig. 3a we have \( T_{12,b}/T_{12,d} \propto \exp \left( -2/\bar{z} \times (R_b - R_d) \right) \). Since \( R_b < R_d \) (see the separation in Fig. 3b and d), this can lead to the transmission ratio of several orders of magnitude due to exponential dependence of \( T_{12,b}/T_{12,d} \) on \( (R_d - R_b) \). Recently, variable range hopping has been reported to be the dominant transport mechanism at low temperatures in large GNRs (\( W > 20 \) nm, \( L > 0.5 \) \( \mu \)m) [29,30]. While in Refs. [29,30] VRH is inferred from temperature dependence of the conductance, here we give evidence of quantum hopping by direct insight into the atomic arrangement of the LDOS.

Fig. 4 shows the transmission functions of all randomly generated GNRs (\( N = 100 \)) for two levels of \( P_{ED} \) (\( a \) and \( b \)), \( P_{V} \) (\( c \) and \( d \)), and \( \delta V \) (\( e \) and \( f \)). The transmission of the ideal GNR and averaged transmissions are also plotted for comparison. Averaged transmission curves show stronger suppression for higher disorder strength. Variability from device to device is high in the case of lattice defects, and relatively low in GNRs with potential fluctuations. As evidenced by a larger spread of transmission curves in Fig. 4b, d and f, the variability is higher for larger defect densities and higher fluctuation amplitudes. Similarly to the discussion about averaged transmissions, the variability of GNRs with potential fluctuations is modest, in fact it is negligible for the realistic \( \delta V \) of 100 mV.

The high transmission variability translates into several important issues. The first problem is that the variation of the ON state current is expected to be very high and it will strongly depend on the supply voltage. For example, in the case of \( P_{ED} = 50\% \) presented in Fig. 4b, the averaged transmission decreases by an order of magnitude if the Fermi level of the ON state is lowered from 1 eV to 0.5 eV. Since the variability is higher at low energies (see the range \( E < 0.7 \) eV for \( P_{ED} = 50\% \) in Fig. 4b), this could be a limiting factor for low supply voltages that are needed for the advanced CMOS nodes and low-power applications. The second important consequence of high transmission variation is the variability of the transport gap, which will be discussed in Section 3.3.

### 3.2. Mean free path in disordered GNRs

In order to study the ballisticity in disordered GNRs, i.e. to find whether the transport is ballistic or scattering-dominated, we calculate the mean free path according to the following expression

\[ \lambda(E) = L \frac{T_{12}(E)}{N_{ch} - T_{12}(E)}, \]

where \( L \) is the nanoribbon length and \( N_{ch} \) is the number of conductive channels obtained from the transmission of the ideal GNR [20].

Fig. 5 shows the energy dependence of the MFP for \( W = 2.58 \) nm and for different \( P_{ED} \), \( P_{V} \) and \( \delta V \) in Fig. 5a–c, respectively. The figure also contains a horizontal dotted line that marks the GNR length \( L = 10.1 \) nm for comparison with the calculated MFP values. The strong transmission suppression in the case of lattice defects is transferred to the behavior of the MFP, i.e. \( \lambda \) decreases for higher disorder and at lower energies. In the case of potential fluctuations, MFP values are almost exclusively higher than \( L = 10.1 \) nm. Moreover, \( \lambda \) exhibits peaks near the transmission steps reaching up to \( \sim 2 \times 10^4 \) nm (\( \sim 20 \) \( \mu \)m) for \( \delta V = 100 \) mV.

The dependence of \( \lambda \) on \( P_{Ed} \), \( P_{V} \) and \( \delta V \) for the 2.58 nm-wide GNR, shown in Fig. 6 for the energy level of 0.5 eV and 1 eV, demonstrates the decreasing MFP with increasing disorder strengths. In the case of lattice defects (Fig. 6a and b), \( \lambda < L \) for all cases meaning that the transport is scattering-dominated. However, Fig. 6c shows that the 2.58 nm-wide nanoribbon with potential fluctuations...


3.3. Variability of the transport gap

Using the obtained transmission curves, we extract the transport gap and its range at $T_{12} = 0.01$ and plot the results, i.e. $E_{\text{ETG}}$ dependence on $P_{\text{ID}}$, $P_{\text{V}}$ and $\Delta V$, in Fig. 8. In the case of edge defects (Fig. 8a), half-gap increases to 0.361 eV for $P_{\text{ID}} = 50\%$, which is an increase of 114% compared to ideal GNR. In contrast to sub-2 nm-wide GNRs investigated in [22], for $W = 2.58$ nm we note a saturation of the $E_{\text{ETG}}$ vs. $P_{\text{ID}}$ curve since the edge-defected GNRs exhibit similar half-gap values. This behavior is a consequence of quantum hopping, as it induces local transmission peaks inside the energy gap, which in turn increases the averaged transmission. The gap values of 0.58–0.72 eV obtained for the 2.58 nm-wide GNR are slightly higher than the experimentally observed energy gaps (~0.4 eV) in 2–3 nm-wide nanoribbons fabricated by unzipping of carbon nanotubes [5], but are much closer than $E_{\text{ETG}}$ predicted by the mobility edge approach [10,25]. Similarly to GNRs narrower than 2 nm, the 2.58 nm-wide GNR also exhibits a monotonic, almost linear, increase of $E_{\text{ETG}}$ with increasing $P_{\text{V}}$ as shown in Fig. 8b. This result indicates that the increased number of vacancies effectively turns off the transmission without transmission-enhancing effects, in contrast to the case of edge defects, due to increasing deficit of atomic sites in the bulk of the nanoribbon. The half-gap equals 0.197 eV and 0.867 eV for $P_{\text{V}}$ of 1% and 10%, respectively, which is an increase of 17% and 413% compared to the ideal GNR. We note that realistic $P_{\text{V}}$ is expected to be <1% and $E_{\text{ETG}}$ enhancement is low in that vacancy density range. Dependence of the half-gap on $\Delta V$ is shown in Fig. 8c and we observe a negligible increase of the half-gap that reaches 0.175 eV for $\Delta V = 500$ mV, i.e. only a 4% increase compared to the ideal GNR.

The range of variation of the half-gap values is indicated by the shaded area in Fig. 8. The variability behaves similarly to the dependence of the half-gap on disorder strength. Namely, the range of $E_{\text{ETG}}$ values in the case of edge defects increases and then saturates as $P_{\text{ID}}$ increases, e.g. the variation is 0.19–0.48 eV for $P_{\text{ID}} = 10\%$ and 0.19–0.70 eV for $P_{\text{ID}} = 50\%$. As for the vacancies, the spread of the half-gap values increases as $P_{\text{V}}$ increases, e.g. the range equals 0.17–0.56 eV for $P_{\text{V}} = 1\%$ and expands to 0.47–1.79 eV for $P_{\text{V}} = 10\%$. In the case of potential fluctuations, noticeable variation of the half-gap is observed only for $\Delta V = 500$ mV, where the highest $E_{\text{ETG}}/2$ is 0.271 eV. The influence of GNR width on the variability of the transport gap is studied for edge-defected GNRs with $P_{\text{ID}} = 50\%$ and widths in the ~1 to 5 nm range. Fig. 9 shows the half-gap dependence on GNR width of the ideal (dashed line) and edge-defected (full line) GNRs. Both curves show an increasing gap values as W scales down. However, edge defects enhance $E_{\text{ETG}}$ considerably and their influence is higher in narrower nanoribbons as can be seen from the increasing separation between the two curves as W decreases. The shaded area in Fig. 9 indicates the $E_{\text{ETG}}/2$ variation and it is evident that the variability of the half-gap also increases in narrower GNRs. In turn, this means that the sub-5 nm-wide GNRs could suffer from a high variation of the OFF state leakage current and a high variability of the gate voltage overdrive that leads to high variation in the ON state as well.

3.4. Variability of the density of states

Fig. 10 presents the influence of disorder on DOS for two edge defect densities (a and b), vacancy densities (c and d) and fluctuation amplitudes (e and f). The DOS curves of all the randomly generated GNRs are shown and compared with the averaged DOS and DOS of the ideal GNR.

In the case of lattice defects, DOS reaches high values inside the bandgap with a maximum at zero energy. This behavior is a consequence of different number of atoms in graphene sublattices caused by random defects, which leads to the existence of

![Fig. 3](image-url)
zero modes for the device Hamiltonian as demonstrated for graphene in [9]. Although it seems natural that the existence of these states should increase the transmission in the OFF state, previous reports have demonstrated that these states are strongly localized [10,22,25], and within the mobility-edge theory they do not contribute to conduction. Nevertheless, the transport can occur via quantum hopping [27–29]. In contrast to lattice defects, potential fluctuations do not induce the DOS peak at $E = 0$ eV and non-zero DOS inside the bandgap is observed only for the high $\delta V$ of 500 mV in Fig. 10f. Therefore, the effect of potential fluctuations on DOS for realistic amplitudes $\delta V < 150$ mV [31,32] is negligible.

The averaged DOS curves closely follow the DOS of the ideal GNR only for low disorder strengths, which is best seen for $\delta V = 100$ mV in Fig. 10e, while edge defects and vacancies cause the smoothing of the Van Hove singularities. For higher disorder strengths, as shown in Fig. 10b, d and f, the average DOS is deformed in comparison with the ideal DOS, i.e. we observe a stronger smoothing of the Van Hove singularities. Interestingly, the averaged DOS becomes almost a linear function of energy for very high densities of lattice defects and fluctuation amplitudes.

The variability of DOS from device to device is very high, as can be seen from the large spread of the DOS curves in Fig. 10. The variability increases as $P_{\text{ED}}, P_{\text{V}}$ and $\delta V$ increase, which is evident if we

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**Fig. 4.** Variability of transmission for two levels of disorder strengths for (a and b) edge defects, (c and d) vacancies, and (e and f) potential fluctuations. Averaged transmission and the transmission of the ideal GNR are given for comparison. $N = 100$ for each disorder case. $W = 2.58$ nm.

**Fig. 5.** Averaged mean free path as a function of energy for the 2.58 nm-wide GNR in the case of (a) edge defects, (b) vacancies and (c) potential fluctuations. The GNR length of 10.1 nm is indicated for comparison (dotted horizontal line). $N = 100$ for each disorder case.
compare the respective plots of Fig. 10, e.g. a and b in the case of edge defects. We note that the Van Hove singularities in DOS of the defected GNRs are generally grouped around the singularities of the ideal GNR. This is more evident in the case of low disorder strength, especially for $d_{V} = 100$ mV in Fig. 10e, while for edge defects and vacancies in Fig. 10a and c, respectively, we observe steps that follow the steps of the ideal DOS. Hence, the averaged DOS does not give proper information about the defected GNRs since they exhibit the Van Hove singularities in the DOS. Therefore, when modeling carrier mobility in GNRs it is more appropriate to find average mobility by averaging the mobilities of GNRs with random DOS curves than by calculating the average mobility using the average DOS obtained by averaging the random DOS curves. Consequently, the high DOS variability caused by disorder will induce high mobility variation from device to device.

3.5. Variability of mobility limited by acoustic phonons

In this work, the variability of mobility caused by the variation of the transport gap and density of states is demonstrated in the case of mobility limited by acoustic phonons (APs). We focus on the effects on DOS and $\mathbf{E}_{\text{TC}}$ caused by edge defects because edge roughness is the dominant disorder in extremely narrow GNRs. The AP-limited mobility ($\mu_{\text{AP}}$) is chosen as it approximately supplies the intrinsic GNR mobility, i.e. the maximum mobility achievable in a device given that all the fabrication-dependent scattering mechanisms, such as line-edge roughness, are minimized.

The calculation of $\mu_{\text{AP}}$ is carried out using the Fermi golden rule, momentum relaxation time (MRT) approximation, with the spinor-like wave-functions for graphene and the perturbation potential for APs taken from [33]. The MRT is obtained as

$$\frac{1}{\tau_{\text{AP}}(E)} = \frac{\pi N_{\text{ph}} D_{\text{AP}} E_{\text{AP}}}{4 \hbar \rho v_{s}^{2}} \varepsilon_{\text{GNR}}(E).$$

where $N_{\text{ph}}$ is the phonon number, $D_{\text{AP}}$ is the deformation potential ($-19$ eV), $E_{\text{AP}}$ is the AP energy ($E_{\text{AP}} = h v_{s} q_{p}$ where $q_{p}$ is the wave-vector in the transport direction), $\rho$ is the mass density ($7.6 \times 10^{-7}$ kg/m$^{3}$), and $v_{s}$ is the velocity of sound in graphene ($2 \times 10^{4}$ m/s). The relaxation rate is proportional to the DOS of the GNR, and inversely proportional to its width, which hints at the strong influence of DOS and $E_{\text{TC}}$ variability on $\mu_{\text{AP}}$. The AP-limited mobility is calculated using the Kubo-Greenwood formula within the MRT approximation, i.e.
\[ \mu_H = \frac{e}{\pi n^2 h v_F} \int_0^\infty v_g(E) f_0\left(\frac{\gamma}{E^2 - (nE_0)^2}\right) dE, \]

where \( v_g \) is the group velocity, \( f_0 \) is the Fermi–Dirac distribution function, and \( N_{inv} \) is the inversion charge density.

The DOS of the ideal armchair GNR is modeled as

\[ g_{GNR}(E) = \frac{n_{sp} l v^2}{\pi^2 h v_F} \sum_{n=0}^\infty \frac{1}{\sqrt{E^2 - (nE_0)^2}} \quad \text{mod}(n, 3) = 0, \]

where \( E_0 \) is the half-gap of the ideal GNR, and only the singularities for which \( \text{mod}(n, 3) = 0 \), i.e., every third is excluded, are accounted for in the DOS as in [33]. The half-gap \( E_0 \) depends on \( W \) and is given by an analytical curve shown in Fig. 11 that is obtained by fitting on the data from the NEGF simulations of ideal GNRs. On the other hand, the DOS of edge-defected GNRs is modeled as

\[ g_{GNR}(E) = \frac{n_{sp} l v^2}{2\pi^2 h v_F} \sum_{n=0}^\infty \frac{E}{\sqrt{2} - (nE_0)^2} \quad \text{mod}(n, 3) = 0, \]

where \( E_0,d \) is the half-gap of edge-defected GNRs. The width-dependence of \( E_{0,d} \) is given by an analytical curve shown in Fig. 11, which is fitted to the NEGF simulation results for edge-defected GNRs with \( P_{ED} = 50\% \). In contrast to (8), all singularities are included in (9) in order to account for the higher number of DOS peaks in GNRs with edge defects reported in Fig. 10a and b. Valley multiplicity equals \( l v = 2 \), while \( n_{sp} = 2 \) when calculating the DOS and \( n_{sp} = 1 \) when calculating the mobility in (6) since the scattering process under study does not flip the spin of the carrier.
For each GNR width, we generate \( N = 500 \) random DOS curves described by (9) in order to find the average mobility that accounts for the effects of edge defects on the DOS and the transport gap. The randomness comes from the variability of the half-gap \( E_0, d \) and the occurrence of additional Van Hove singularities in the DOS of edge-defected GNRs. The standard deviation of \( E_0, d \) is obtained from the NEGF results in Fig. 9, and the analytical curve for the deviation of \( E_0, d \) is plotted in Fig. 11.

All AP-limited mobility curves \((N = 500)\) and the averaged mobility for \( W = 2.58 \) nm are reported in Fig. 12a, where \( \mu_{AP} \) obtained for the ideal 2.58 nm-wide GNR is also shown for comparison. We observe a high variation of \( \mu_{AP} \), from \( \sim 700 \) cm\(^2\)/Vs up to \( \sim 6900 \) cm\(^2\)/Vs with the averaged \( \mu_{AP} \) being \( \sim 3000 \) cm\(^2\)/Vs at \( N_{inv} = 10^{12} \) cm\(^{-2}\). Therefore, the high variability of the transport gap caused by edge defects translates into high variability of the low-field AP-limited mobility. The same is expected for other important scattering mechanisms as well, i.e. optical phonon, line-edge roughness, Coulomb scattering, since the scattering rates depend directly on the DOS [25,33,34]. The detrimental influence of defects is also seen in the fact that the averaged mobility of realistic GNRs is \( \sim 2 \times \) lower than the mobility of the ideal 2.58 nm-wide GNR, i.e. 2990 cm\(^2\)/Vs compared to 5840 cm\(^2\)/Vs at \( N_{inv} = 10^{12} \) cm\(^{-2}\). Dependence of the averaged mobility on \( N_{inv} \) for GNR widths form 1.10 nm to 4.80 nm is presented in Fig. 12b and c, for the ideal and defected GNRs, respectively. Generally, the shape of the mobility curve is preserved when defects are accounted for, while the defected GNRs exhibit average mobilities that are lower than the mobility of their ideal counterparts and the difference is larger for narrower nanoribbons.

Fig. 13 presents the influence of GNR width downscaling on the mobilities of ideal and edge-defected GNRs. The shaded area shows the variation of \( \mu_{AP} \) in defected GNRs obtained by simulation of \( N = 500 \) for each defected nanoribbon.

![Fig. 12. (a) Variability of \( \mu_{AP} \) in the 2.58 nm-wide GNR. The averaged \( \mu_{AP} \) and \( \mu_{AP} \) of the ideal GNR are also shown. Mobility vs. charge density for various GNR widths is shown in (b) for the ideal GNRs and (c) for GNRs with edge defects. Averaged \( \mu_{AP} \) in (c) are obtained by simulating \( N = 500 \) devices for each GNR width.](image)

![Fig. 13. Influence of GNR width downscaling on the AP-limited mobility in the ideal and edge-defected GNRs. The shaded area shows the variation of \( \mu_{AP} \) in GNRs with edge defects. \( N = 500 \) for each defected nanoribbon.](image)

4. Conclusion

We have employed atomistic NEGF simulations and semiclassical mobility simulations of large ensembles of devices in order to investigate the transport properties of sub-5 nm-wide GNRs. With increasing disorder strength the suppression of the averaged transmission becomes stronger, except in the case of edge defects where a saturation is observed due to quantum hopping that enhances the transmission inside the energy gap. In edge-defected GNRs...
with $\phi_{FD} = 50\%$, $E_{FC}/2$ increases from 0.106 eV to 1.709 eV when $W$ is scaled down from 4.80 nm to 1.10 nm. For the same GNR width range the standard deviation of the half-gap increases from 37 meV to 223 meV. The investigation of the MFP in the 2.58 nm-wide GNR has revealed that the transport is scattering-dominated in the case of lattice defects, whereas $\lambda > L$ is obtained in the case of potential fluctuations, which indicates ballistic transport. Similarly to the transmission and $E_{TC}$, the variation of the MFP is also very high. The MFP remains smaller than $L$ in edge-defected GNRs with the widths of 1.10–4.80 nm, ranging from $\sim 8$ nm down to $\sim 10^{-4}$ nm. Based on the data obtained from the NEGF simulations, we propose an analytical model for the DOS of disordered GNRs and calculate the AP-limited mobility. The model accounts for the increased $E_{TC}$ in edge-defected GNRs, for the variation of $E_{TC}$, and for the occurrence of additional Van Hove singularities in the DOS of edge-defected GNRs. We report the high $\mu_{AP}$ variation, e.g. for $W = 2.58$ nm the range equals 700–6900 cm$^2$/Vs with the averaged $\mu_{AP}$ being $\sim 3000$ cm$^2$/Vs at $N_{inv} = 10^{12}$ cm$^{-2}$. Wider GNRs exhibit $\mu_{AP}$ similar to those of the respective ideal GNRs, while the $\mu_{AP}$ vs. $W$ curves of ideal and defected devices diverge as the width scales down. For example, the averaged $\mu_{AP}$ of the 2.58 nm-wide GNR is $\sim 2 \times$ lower than the AP-limited mobility of the ideal counterpart. The high variability of transport properties in sub-5 nm-wide GNRs, observed from the transmission and transport gap to the DOS and mobility, could be the red brick wall for GNR applications in nano electronics.

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