Monte Carlo study of velocity fluctuations during transient regimes in graphene

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I. INTRODUCTION

Graphene is a two-dimensional carbon allotrope consisting of a single-atom-thick sheet of carbon atoms arranged in a hexagonal lattice. Its remarkable properties have made it become, in the recent years, one of the most fashionable materials among the industry and researchers due to its promising aptitudes for a lot of electronics and optoelectronics applications[1–3]. The above described crystalline structure gives rise to an unusual gapless conic-shaped dispersion relation in the vicinities of the six K points (i.e. the six points in the Brillouin zone where $E_F = 0$) which is of tremendous interest for being the origin of the massless behaviour that electrons exhibit in this material[4]. The most direct implication of this feature is that electrons in graphene travel with a constant velocity called the Fermi velocity, $v_F \approx 10^6$ cm s^{-1}, and therefore carrier velocity along a certain direction depends only on its wavevector orientation: $v_x = v_F \frac{k_x}{|\vec{k}|}$. As a result, velocity fluctuations in graphene are limited[5] to a maximum value of 2 v_F and velocity relaxation through scattering mechanisms depends only on the momentum orientation, and it is strongly affected by the anisotropy of the scattering mechanisms.

For most of the practical uses, graphene is not used as separated sheets, but attached to a substrate layer. The presence of a substrate affects the graphene performance[6] by degrading the carrier mobility velocity and diffusion coefficient at low fields but increasing the saturation velocity. In this work, we will assess the influence of h-BN and SiO_2 substrates in the transient regime velocity fluctuations compared to the ideal monolayer suspended graphene.

As a result of the above mentioned interest in this material, several works regarding noise in graphene devices have been carried out[7–10]. With the purpose of offering a miscroscopic study of the inherent sources of noise in the material, we present a study of instantaneous velocity fluctuations in graphene by means of computational simulation performed with the Ensemble Monte Carlo Method. Our simulator takes into account the massless Dirac Fermions behaviour related to the linear dispersion relation. Pauli exclusion principle is implemented through a rejection technique after each scattering event. The scattering sources taken into account in our simulations are optic, intravalley and intervalley acoustic phonons, and surface polar phonons in case of graphene on a substrate[11,12]. In addition, we include in this work the effect of elastic scattering with charged impurities, considering a density $n_{imp} = 5 \times 10^{11}$cm^{-2} in both suspended graphene and graphene on a substrate. Given the importance of all these interactions in the velocity fluctuations, along with the strong dependence of velocity with the wavevector orientation, the anisotropy of all these scattering mechanisms is treated rigorously.

In previous studies we have used Monte Carlo simulations to examine velocity fluctuations in graphene[13] and diffusion coefficients were calculated from the correlation function of velocity fluctuations[5,11]. However, when devices work under switching conditions, the carriers are not usually in a steady state, but in a transient situation of change towards the final stationary state associated with the applied electric field. In this work we offer an in-deph study in the transient regime of the velocity fluctuations for suspended graphene and graphene on a substrate. For this, we set transient regimes for low to high electric fields and vice versa. In the case of graphene, due to its high mobility, we chose the low field value so that it is away from the values that produce the saturation velocity. The quantities to be analysed are the transient correlation function and spectral density of velocity fluctuations, which are calculated from the Monte Carlo simulator as follows. The instantaneous velocity fluctuation for a single electron, is $\delta v(t) = v(t) - \langle v(t) \rangle$, where the brackets indicate the ensemble average. The autocorrelation function keeps its traditional definition[5]. On its behalf, since the study of velocity fluctuations is performed over finite times during the transient, the spectral density cannot be obtained as the Fourier transform of the autocorrelation function.[14] Instead, it is calculated at different times with the expression $S_{\delta v}(f, \tau) = \frac{1}{\tau} \left\langle \left| \int_0^\tau \delta v(t) e^{j\omega t} \, \mathrm{d}t \right|^2 \right\rangle$.

II. RESULTS

In Fig. 1 we show the averaged ensemble velocity during the transient from low to high field and vice versa. For the low to high field leap (Fig. 1-a) stationary velocity is reached in a sub-ps time scale. The velocity overshoot is less pronounced in the graphene on a substrate than in suspended samples. It is to highlight the difference in the transient times, that are much longer in high to low field transitions. For the high to low field transient (Fig. 1-b) the trend of the saturation velocity is different if we compare the suspended graphene to graphene lying on a substrate. In the suspended case, the transient velocity experiments an intense drop until

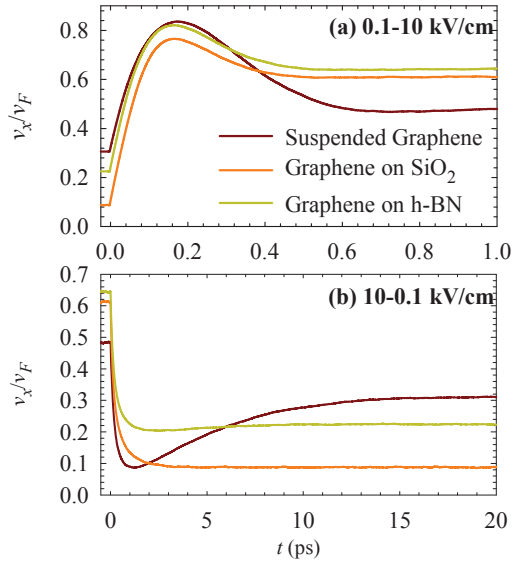

FIG. 1. Time evolution of the averaged ensemble velocity for suspended and supported graphene. The transients are (a) 0.1 to 10 kV cm^{-1} and (b) 10 to 0.1 kV cm^{-1}

reaching a minimum at $t \approx 1$ ps and afterwards there is a progressive increase until reaching the stationary state at around 15 ps. For graphene on a substrate, the steady state velocity for 0.1 kV cm^{-1} is reached in less than 5 ps, being the local minimum totally absent when the substrate is SiO_2 and almost inappreciable if it is h-BN.

Fig. 2 depicts the 0.1 to 10 kV cm^{-1} transient spectral density for various instants for suspended graphene (a) and graphene on SiO_2 (b). The qualitative evolution is quite similar. In the two cases the spectral density starts with similar values. Then, progressively it evolves towards the 10 kV cm^{-}1 stationary spectral density, increasing in the frequencies ranging from 500 to 3000 GHz, where there is a maximum, and decreasing less prominently in the rest of the frequency range considered.. In suspended graphene the maximum is already perceptible at 0.25 ps and shifts towards lower frequencies for the successive intervals. With regard to the SiO_2 sample, the maximum persists around the same frequency for all the intervals considered.

In the conference a deeper study will be offered from the analysis of the microscopic information extracted from the Monte Carlo simulations together with the transient correlation functions and the spectral densities.

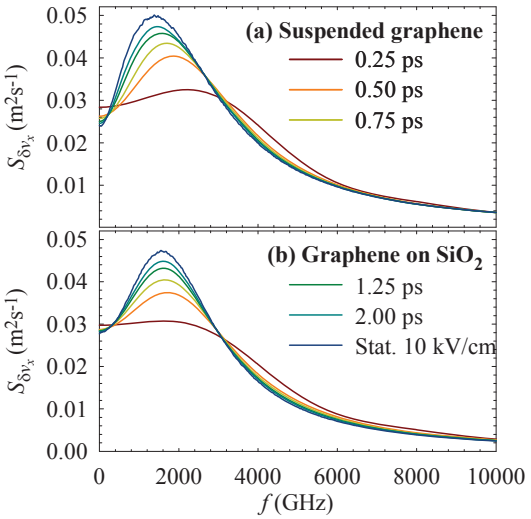

FIG. 2. 0.1 to 10 kV cm^{-1} transient spectral densities for various instants in (a) suspended graphene, and (b) graphene on SiO_2

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