Impact of the Temperature and Remote Phonon Scattering on Charge Transport in Supported Graphene

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Graphene is an exciting material with electrical properties outperforming those of conventional semiconductors. For example, suspended monolayer graphene presents a much elevated intrinsic mobility at room temperature as compared to Si or III-V materials [1], which has been an important incentive for exploring the use of graphene in future electronic devices. In real samples, however, the presence of a supporting dielectric material may significantly degrade the electrical characteristics of graphene [2], although still a great advantage is obtained as compared to traditional semiconductors.

In this work, we present an investigation of the temperature dependence of parameters such as the resistivity, saturation velocity or diffusion coefficient in suspended monolayer graphene and graphene on several types of substrates (e.g., h-BN, SiC, SiO_2 and HfO_2). The results have been obtained by means of an ensemble Monte Carlo (EMC) simulator. EMC simulators have previously shown their utility for an in-depth description of the electrical charge transport parameters in graphene [3-5]. The scattering mechanisms considered in the present work are intrinsic optical phonons, intervalley and intravalley acoustic phonons and surface polar phonon (remote phonon) scattering, or SPP. Impurities or defects are not taken into account in order to provide an adequate insight of the influence of the phonon scatterings related to the substrate type. The diffusion coefficient D is obtained by means of the analysis of the second central moment of the ensemble of particles diffusing across the material, and also from the Fourier analysis of velocity fluctuations, following the methodology described in [5]. The procedure involves the consideration of an excess carrier population evolving according to a linearized Boltzmann transport equation, since the material is considered to be degenerate at low fields for the carrier concentration simulated (10^{12} cm^{-2}); more details can be found in previous works [5,6].

The DC resistivity (obtained from the velocity-field curves at a small applied field equal to 10 V/cm) and the diffusion coefficient as a function of the temperature are shown in Figure 1. Excellent agreement with the resistivity results by other authors [3] (shown in the graph for the case of SiO_2) is observed. As expected, at room temperature suspended graphene shows the largest diffusivity and lowest resistivity values, well beyond those obtained for supported samples. However, as the temperature is lowered, the differences tend to reduce. For example, suspended graphene and graphene on h-BN or SiC show similar D and resistivity values for temperatures below 175K, and graphene on SiO_2 gets close also for $T < 100K$ (and so do the mobility values, not shown in the graphs), which is strongly related to the behaviour of SPP interactions, as it will be discussed later. The anisotropic nature of SPP interactions yields larger saturation velocities as compared to the suspended case at 300 K [6], which are maintained also for lower temperatures, with the only exception of HfO_2 (Figure 2(a)) for which the remote phonon activity is extraordinarily large due to the small phonon energies in that case. Negative differential conductivity (NDC) was clearly evidenced in all cases, with the exception of graphene on HfO_2, for which only a small NDC was obtained at very high fields. NDC becomes more evident at low temperatures (Figure 2(b)). It is important also to notice the augmentation of the scattering time at low temperatures, particularly for graphene on SiO_2

(Figure 3(a)). In general, there is an important reduction of the SPP activity at low temperatures, as evidenced in Figure 3(b), which explains that, in an ideal framework absent of impurities and defects, for temperatures in the range of 100K and below graphene on h-BN, SiC or SiO_2 have comparable electrical characteristics to those of suspended graphene.

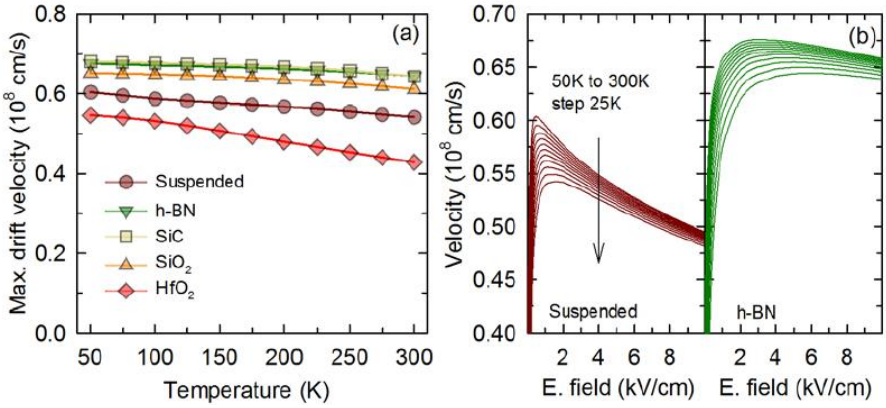

Figure 2. Maximum drift velocity for suspended graphene and graphene on different types of substrates (a). Velocity-field curves for suspended graphene and graphene on h-BN (b).

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References

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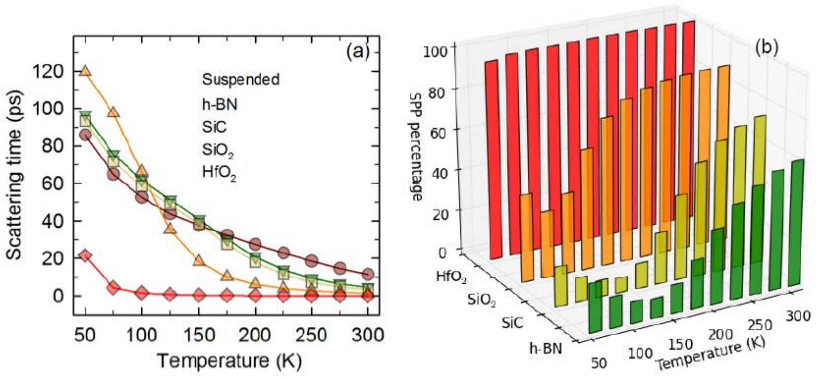

Figure 3. Scattering time at an applied field equal to 10 V/cm (a) and percentage of SPP scattering mechanisms over the total number of scatterings in graphene on h-BN. SiC, SiO_2 and HfO_2 (b).

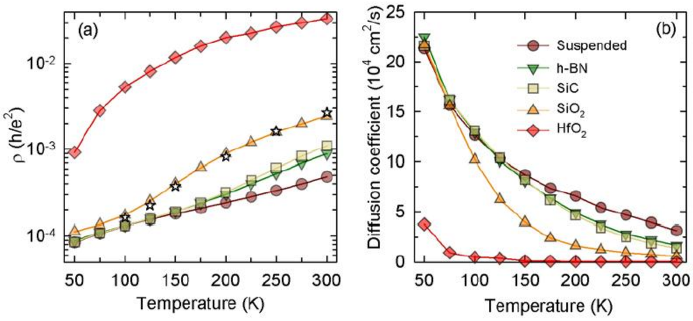

Figure 1. DC resistivity (a) and diffusion coefficient (b) as a function of the temperature for suspended graphene and graphene on different types of substrates. The carrier concentration is 10^{12} cm^{-2}. The white stars in (a) show values for SiO_2 from reference [3].