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Effect of charged impurity scattering on the electron diffusivity and mobility in graphene

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Abstract. The influence of charged impurities on the transport properties of graphene, including the diffusion coefficient at low and high electric fields, is investigated by means of an ensemble Monte Carlo simulator. Three different possible substrates are considered, h-BN, SiC and SiO_2. The results show the importance of impurity scattering in degrading the diffusion coefficient, electronic mobility and drift velocity, particularly at low and intermediate electric fields. The influence of the substrate dielectric constant in relation to impurities and surface polar phonon scattering is also evidenced; this turns SiC into the most suitable substrate of choice from this point of view.

1. Introduction

Graphene is commonly recognized as one of the most promising materials for future electronics [1]. However, its excellent intrinsic electronic properties are significantly affected by several effects appearing in fabricated samples. In particular, Coulomb impurities acting as long-range scatterers are an important scattering source in graphene, limiting the conductivity in this material [2]. Therefore, it is of primary importance to consider this type of interaction in realistic models for the study of graphene. Moreover, it becomes particularly interesting to analyze the interplay of this kind of scattering with intrinsic phonon interactions and with remote phonons from the underlying substrate, and to study how the substrate type affects the Coulomb screening of the charged impurities.

In this work, we have analyzed the influence of charged impurities on the transport properties of graphene, including the low-field mobility and the diffusion coefficient at low and high electric fields, by means of an ensemble Monte Carlo simulator. For relatively high carrier concentration, slightly away from the Dirac point, the semiclassical Boltzmann transport theory provides a good description of charge transport physics in graphene [3]. Consequently, the Monte Carlo method becomes a powerful tool for the investigation of the electronic transport properties of this material [4]. Three different substrates have been considered, i.e., h-BN, SiC and SiO_2.

2. Monte Carlo simulator

The calculations have been carried out by means of an ensemble Monte Carlo simulator incorporating the main properties of graphene, such as a linear dispersion relation close to the Dirac point, which implies that electrons behave as massless particles. The most relevant scattering mechanisms are included in the simulation [5, 6].

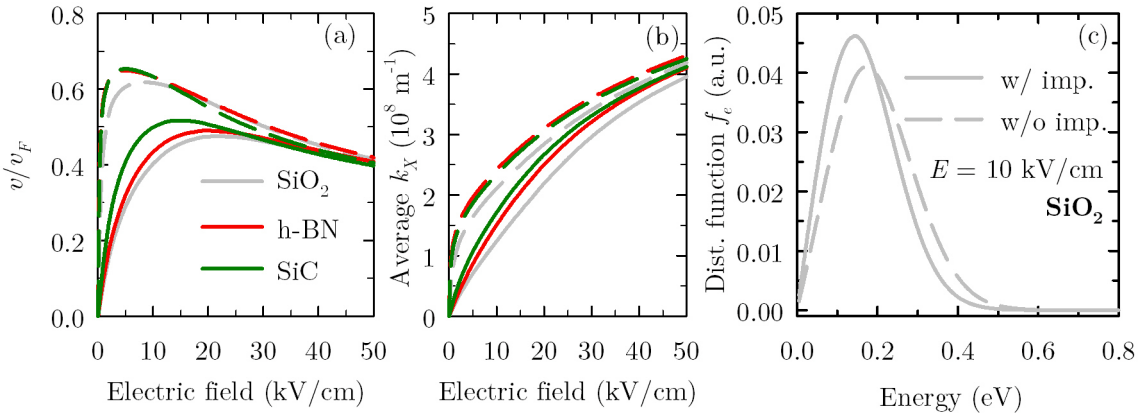

Figure 1. Average drift velocity (a), average wavevector in the direction of the applied field (b) and energy distribution function for the case of SiO_2 (c). Solid lines represent the results including impurity scattering and dashed lines without it. The electron density is 10^{12} cm^{-2}.

In the case of Coulomb interactions with charged impurities, the scattering matrix element is obtained from the 2D Fourier transform of the electrostatic potential [2, 3, 7]. Applying Fermi's Golden rule it is possible to obtain the transition probability as a function of the energy, which is proportional to the impurity density. The anisotropy of Coulomb scattering is rigorously treated for the selection of the final angle after a scattering event.The screening of 2D Coulomb interactions is included taking into account its anisotropic nature and the static polarizability to account for the dielectric function [8], considering the electronic temperature self-consistently determined at each timestep [9]. The calculation of the diffusion coefficient is carried out as explained in [5], considering an excess electron population coupled to the background population by means of a carrier-carrier exchange scattering mechanism.

3. Results and discussion

The effect of charged impurities on the electron drift velocity as a function of the applied field is shown in Figure 1(a). The electron density concentration considered in this work is equal to 10^{12} cm^{-2}. The impurity density is $5{\cdot}10^{11}$ cm^{-2} for all the substrates under study. As it can be observed, impurities noticeably reduce the drift velocity, particularly at low and moderate (below 20 kV/cm) electric fields, and they also moderate the negative differential conductance observed.

At very high fields the differences tend to reduce, not only between the case with and without impurities, but also in relation to the different substrate types. It is interesting to remark that, while in the absence of impurities graphene on h-BN and on SiC present similar velocity peak values, when impurities are considered graphene on SiC clearly outperforms graphene on h-BN. The average wavevector in the direction of the applied field is shown in Figure 1(b). Charged impurity scattering reduces the average wavevector value, with the largest influence in the range 0-10 kV/cm. This is directly related to a reduction in the average energy provoked by this kind of interaction; it also shifts the energy distribution function f_e, as evidenced in Figure 1(c), which shows f_e at 10 kV/cm for the case of considering SiO_2 as the supporting substrate. A similar behavior of f_e for h-BN and SiC was observed.

In order to discuss the influence of charged impurity scattering, it is relevant to check the quantitative influence of this type of interactions as compared to other scattering events in the graphene layer. Figure 2 shows the average number of scattering events per unit time for the three cases under consideration (graphene on SiO_2, on h-BN and on SiC). The maximum

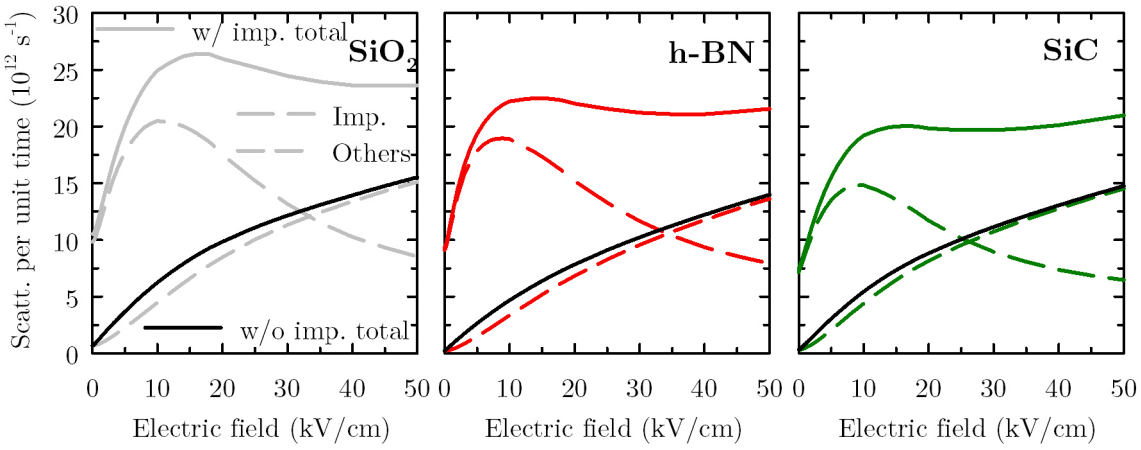

Figure 2. Average number of scatterings per unit time, for SiO_2 (a), h-BN(b) and SiC (c). 'w/imp total' refers to the total number of scatterings when impurities are included and 'w/o imp total' the total number when impurities are not considered.

intensity of impurity scattering is obtained for electric fields close to 10 kV/cm in all cases; it is also noticeable the reduced influence of impurity scattering in the case of SiC. This is related to the larger dielectric constant of this substrate type, which provides a more intense screening of the impurities and therefore reduces the strength of this interaction. Due to the reduction of the average energy in the presence of charged impurities, the other types of scattering events have a reduced rate as compared to the case without impurities. At very high electric fields, over 10 kV/cm, the influence of impurity scattering becomes progressively reduced: its Coulomb nature makes it less prone to affect electronic transport at high energies.

Charged impurity scattering also affects to how much power is transferred to the graphene layer and the underlying substrate via inelastic phonons (Figure 3(a)). Below 10 kV/cm, there is a significant reduction of the power exchange due to inelastic interactions, which would translate into less self-heating in the samples.

Let us now check the evolution of macroscopic parameters as the low-field mobility or the diffusion coefficient as a function of the impurity concentration (Figures 3(b) and 3(c)). In the absence of impurities, graphene on h-BN provides the best results (mobility equal to 260,000 cm^2/Vs, diffusion coefficient equal to 15,800 cm^2/s), with graphene on SiC closely following (221,000 cm^2/Vs and 13,200 cm^2/s) and graphene on SiO_2 clearly underperforming (96,500 cm^2/Vs and 5,800 cm^2/s). However, when impurities are present, this behaviour changes: both parameters are significantly reduced (one order of magnitude approximately) and graphene on SiC shows the best performance of the cases under study, with graphene on h-BN only slightly better than graphene on SiO_2. This is directly related to the lower dielectric constant of h-BN as compared to SiC, which affects the screening of impurities and surface polar phonon scattering.

At high fields (over 10 kV/cm) the diffusion coefficient presents similar values for all the substrates under consideration. In this case, even so if charged impurities are still the dominant scattering type, its strong anisotropic nature and the large energy values attained in this rage moderate their influence on the microscopic diffusion processes.

The high-field drift velocity at 10 kV/cm (Figure 3(d)) also shows important differences, with SiC also presenting the largest values as compared to the other substrates under consideration. This is clearly related to the reduced influence of impurities in this case, as previously discussed. However, at very intense fields (50 kV/cm) the differences tend to reduce, as inelastic scattering processes tend to minimize the differences between the different cases under consideration.

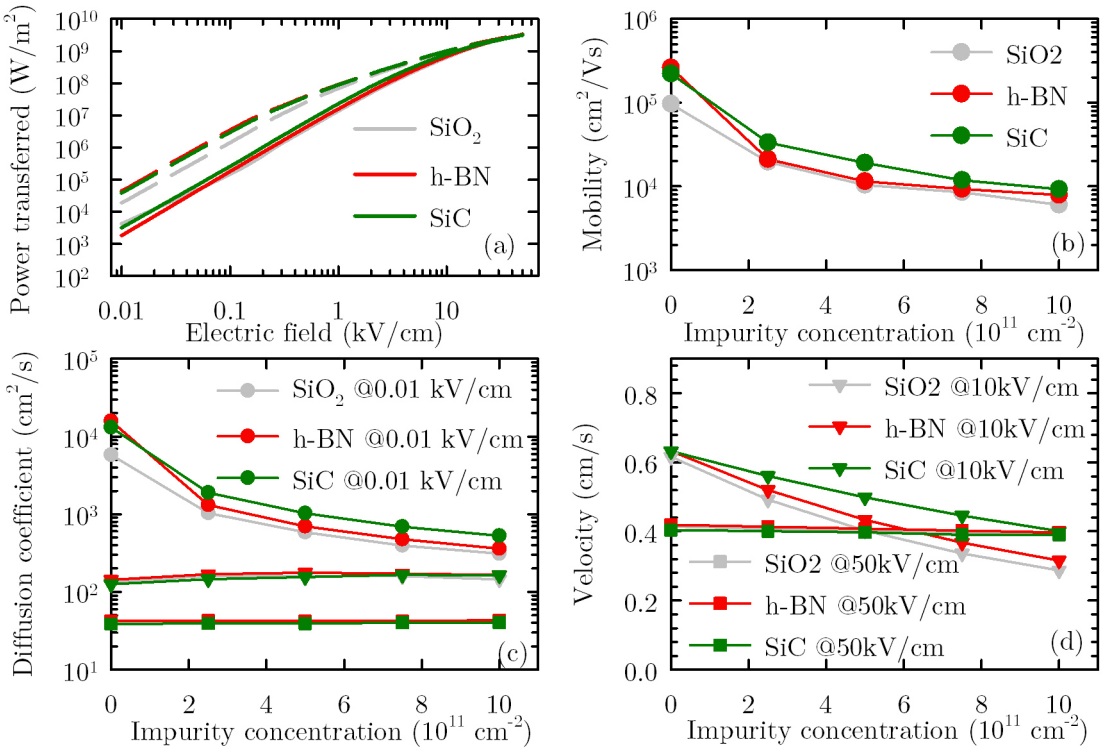

Figure 3. Power transferred as a function of the electric field (a), low-field mobility as a function of the impurity concentration (b), diffusion coefficient (c) and high-field drift velocity (d).

4. Conclusions

The influence of charged impurities on macroscopic parameters such as the low-field mobility, diffusion coefficient or drift velocity has been analyzed by means of a microscopic ensemble Monte Carlo approach. The results evidence that charged impurities significantly affect the transport properties of graphene on a substrate, degrading the overall performance. Moreover, the substrate type is of key importance: in the absence of impurities graphene on h-BN shows the best performance, while in the presence of impurities graphene on SiC gives the best results in terms of drift velocity, low-field mobility and diffusion coefficient, due to a more efficient screening of charged impurities.

Acknowledgments

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