Room temperature velocity saturation in intrinsic graphene

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Room temperature velocity saturation in intrinsic graphene

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Abstract. We report ensemble Monte Carlo (EMC) studies of velocity saturation in intrinsic graphene at room temperature. The parameters for the phonon scatterings were obtained from fitting experimental data of graphene sheets in a variety of dielectric media, in which mobilities as high as 44,000 cm²/Vs were observed at 300 K. In our work, velocity saturation was clearly observed at low carrier density (≤5×10¹² cm⁻²). Saturation velocity as high as 5.4×10⁷ cm/s was achieved at the lowest density (5×10¹¹ cm⁻²). Only scatterings due to the acoustic phonon and the K-point intervalley optical phonon were considered in the simulation. As the density increases, the onset value increases and the saturation velocity decreases.

1. Introduction

Graphene is one of the most notable discoveries made in last century. Although scientists have been investigating graphene for nearly seven decades, it became a serious topic after 2004 when A. Geim and his group were successfully able to extract graphene in its two-dimensional form by mechanical exfoliation [4]. After that a great deal of interest both in theoretical and experimental fields initiated for investigating the electronic properties of two dimensional graphene [5]. Graphene is a strictly two-dimensional material which has excellent high crystal and electronic quality and despite being a new comer, it presented itself as a promising material for future nanotechnology. Graphene is indeed an extraordinary material having unusual behavior which distinguishes it from other two dimensional semiconductor systems. In its single layer form, graphene is only one atom thick sheet of carbon atoms where the atoms are arranged in a honeycomb shape. It has unique bandstructure where the bands and electron transport are mainly influenced by the linear energy bands near the Dirac point [6]. The band structure itself is governed by the Dirac equation, in which charge carriers imitate relativistic particles with zero rest mass.

In order to utilize graphene in coming nanoscale devices, its high field behavior must be investigated thoroughly. Since the first studies into the breakdown and current saturation in semiconductors, the hot electron behavior is of great interest among the researchers [7,8]. It appears that at high electric fields, only the strong metals are able to maintain linear behavior [9]. But, graphene is a strange metallic material, with somewhat conflicting device characteristics. Although intense theoretical studies are carried on graphene’s transport [10,11,12,13,14], however, there have been apparently no reports of high electric field behavior in intrinsic graphene to date. Lin et al., observed little effect of the gate in graphene field effect transistors [15] which was expected from the Klein paradox where electrons tunnel through finite length barriers without reflection [16]. But Meric

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et al. found contradictory results in their experiments. They observed current saturation in similar transistors as expected by electrostatic depletion from the gate [17]. While they considered the possibility of velocity saturation, which is present in carbon nanotube, not much is presently known about this phenomenon in graphene [18].

In this paper, we conduct a systematic study of velocity saturation in graphene as a function of electron density and electric field. For this purpose we employed an ensemble Monte Carlo procedure to solve the Boltzmann transport equation with the unique graphene band structure. In order to determine the drift velocity in any material, usually the value of mass is required. For graphene, away from the Dirac point, the mass is found easily by relating the particle momentum to the crystal momentum. This rather unusual way of determining mass yields a result that is the same as the cyclotron mass where it varies linearly with momentum [19]. Therefore, we calculate the drift velocity in graphene from the following relationship

\[ v_d = v_F \langle \frac{k}{k_F} \rangle, \] (1)

where \( v_F \) is the Fermi velocity and the angular brackets denote the ensemble average.

2. The transport model

For this paper, our interest lies only in the velocity behavior which is limited by intrinsic phonon in graphene at room temperature. So far most of the room temperature transport studies addressed limited mobility due to the impact of impurities in the SiO_2 upon which the exfoliated graphene is deposited. Recently, this situation changed when single layer graphene samples were immersed in various high K dielectric solvent in order to screen the effect of charged impurities which resulted in very high mobilities at room temperature [20]. Charged impurity scattering is the most dominating scattering mechanism in graphene at low density. When its effect was drastically reduced by these strong polar solvents, graphene’s mobility was basically determined by the intrinsic phonon scattering. This helped
us to separate the intrinsic mobility at various densities and moreover, allowed us to determine the coupling constant for the acoustic phonons as well as to estimate the coupling constant for the optical phonons. Here, we include only these scattering mechanisms in the calculation. The optical phonon scattering is by $K$ point phonons which couple the two equivalent valleys of the conduction band. From studies of the phonon structure, this is the LA+LO mode with an energy of 150 meV [21]. Detailed derivations for the scattering rates are given elsewhere [22].

3. Results

Fig 1 illustrates the mobility for high $K$ dielectric solvent ($K=47$ and $K=66$) along with the theoretical intrinsic mobilities calculated using different coupling constants. We can see the best set of values to fit the experimental results are $D = 14$ eV for the acoustic modes and $D_0 = 4.1 \times 10^9$ eV/cm for the optical mode. As mentioned above, these values lead to a room temperature mobility above 40,000 cm$^2$/Vs in what is believed to be intrinsic graphene. Although these coupling constants provide very good fit for the low density regime of the data, the theoretical curve lies above the measured data at high density region. Although we currently do not have full understanding about this discrepancy, but low energy phonon modes that are accompanied by high dielectric constant may be the reason for mobility degradation at higher density. However more work need to be done to confirm this statement. It is important to note that these coupling constants are not unique. Calculation with different coupling constants obtained from the same set of data has also been published [23].

In Fig. 2, we plot the steady state drift velocity as a function of applied field for different carrier densities. The onset of saturated behavior is found to occur at lower field but the velocity gets higher with lower carrier density which is indeed remarkable. Because of graphene’s unusual linear dispersion relation near the Dirac point, both the energy and the mass increase linearly with total momentum. At lower carrier density, scattering increases but mass decreases and both of them contribute for velocity increment. The ratio of average energy to the Fermi energy is plotted against the electric field in Fig 3 for different densities. At low electric field and high density, the ration is very close to 0.67 which is expected for degenerate electron gas in graphene at equilibrium. In Fig. 4, the velocity at 30 kV/cm is plotted as a function of the average energy attained at the field. It is easily

![Figure 2](image)

**Figure 2.** The steady state velocity as a function of applied electric field for different carrier densities.
observable that there is an inverse square relationship present between the average energy and the velocity. Incidentally, this is not unexpected at all for graphene. At any value of the field, there is an effective mobility relating the velocity to this field, as

\[ v = \mu F = \frac{e \tau F}{m} \]  

Here \( \tau \), the relaxation time, is inversely proportional to the density of states and also to energy. Again, the effective mass increases linearly with energy for graphene. Because of these, it is expected, to first order, that the velocity will decrease with the square of the energy, and this is very nearly the situation found in Fig. 4.

Finally, in Fig. 5, we illustrate how the initial Fermi-Dirac distribution is broadened and shifted in the high electric field. This confirms that there is a change in both the average energy (change in the Fermi energy) and in the temperature (broadening of the distribution) as the field is increased.

4. Conclusions
We have studied the transport of energetic electrons in graphene at room temperature. anomalous velocity saturation, that is velocity saturation behavior different than observed in normal semiconductors, is observed in intrinsic graphene at room temperature when only phonon scatterings are considered. The reason behind this anomaly lies in graphene's unique bandstructure which has a linear dispersion relation near the Dirac point. The saturated velocities showed systematic variation with both the average energy and the carrier density. We also find that the value of the saturation velocity is a function of the electron density itself, with strong saturation being observed only at low density.
Figure 4. The steady state drift velocity at 30 kV/cm applied field as a function of average energy for carrier density, \( n_s = 5 \times 10^{12} \text{ cm}^{-2} \).

Figure 5. The Fermi-Dirac distribution at three different electric fields for carrier density, \( n_s = 5 \times 10^{12} \text{ cm}^{-2} \).

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