MONTE CARLO STUDY OF IONIZED IMPURITY SCATTERING IN QUANTUM WIRES

Lucio Rota
Clarendon Laboratory, Department of Physics
University of Oxford, Parks Road, Oxford OX1 3PU, UK

Stephen M. Goodnick
Department of Electric and Computer Engineering
Oregon State University, Corvallis, Oregon, 97331

Abstract

We have developed a multi-subband Monte Carlo simulation of nonequilibrium transport in quasi-one-dimensional AlGaAs/GaAS quantum wire systems. The simulation includes scattering due to confined polar optical phonons, carrier-carrier scattering, and scattering due to elastic mechanisms such as boundary roughness and impurity scattering. In the present work, we present a detailed Monte Carlo investigation of the effect of ionized impurity scattering in quantum wires under an applied electric field. Static screening in the long wavelength limit is assumed using the multisubband RPA dielectric function for the quasi 1D system. We studied separately the effect of uniformly distributed impurities in the wire and of remote impurities. The former strongly affects transport, particularly at low electric fields and at low temperature. The effect of remote doping is much weaker and practically negligible at room temperature.

I. INTRODUCTION

Recent advances in nanostructure semiconductor technology have allowed the fabrication of wire-like structures where quasi one-dimensional confinement is achieved in a semiconductor material surrounded by another semiconductor with larger band gap [1]. In particular, such wire-like structures have been fabricated with rectangular cross sections [2]. In general, carrier dynamics in wires may be expected to differ from the bulk case: the carrier-phonon scattering rate is affected by changes in the electronic [3] and vibrational [4] properties induced by reduced dimensionality. In the last few years a lot of attention has been dedicated to the study of the electron-phonon interaction in these systems [3-7]. This is certainly the more important interaction and almost the only one present if we are interested in the optical properties of wires. On the other hand, if we hope to be able to take advantage of the reduced 1D density of states to produce electronic devices with higher mobility, the electron-impurity interaction must be seriously considered. The aim of this work is to accurately study the effect of this interaction in quantum wires through a Monte Carlo simulation [8].

II. THEORY

We start by considering the bare unscreened interaction with an impurity located in the point (X, Y, Z), the matrix element is given by:

$$H(q_x) = \langle \Psi_i(x,y,z) \mid H \mid \Psi_j(x,y,z) \rangle = \frac{e^2}{4\pi\epsilon} \int dz \int dy \phi_i(y,z) \phi_j^*(y,z) \cdot$$

$$\frac{1}{L} \int dx \frac{e^{-i(k_x - k_x')x}}{\sqrt{(x-X)^2 + (y-X)^2 + (z-Z)^2}} =$$

$$\frac{e^2 e^{-iq_x X}}{2\pi\epsilon L}\int dz \int dy\,\phi_i(y,z)\phi_j^*(y,z)K_0\left(\mid q_x \mid \sqrt{(y-Y)^2+(z-Z)^2}\right) , \tag{1}$$

where $q_x = k_x - k_x'$. The total scattering rate for a carrier in a given subband i and with a given wave vector k_x is the sum over all available final states:

$$\Gamma(i,k_x) = \frac{e^4}{4\pi^2\epsilon^2\hbar^3 L}\sum_j \left[\frac{m_j}{\mid k_x' \mid}\left(\mid H(k_x - k_x') \mid^2 + \mid H(k_x + k_x') \mid^2\right)\right] . \tag{2}$$

This is the probability for an electron to interact with one impurity. If n_I is the linear density of impurities in the wire, we generate in our simulator their position randomly and then we sum over all the impurities to compute the total scattering rate. In the present work, we used a randomly uniform distribution in the three spatial directions, although the model can handle any profile distribution in the same way. The sum over j in Eq. 2 represent the sum over all possible final subbands. For each final subband there are only two contributions, forward $(k_x - k_x')$ and backward $(k_x + k_x')$ scattering. When the initial and the final subbands are the same, only the backward scattering remains. Looking at Eq. 2 we can also draw some initial conclusions: As in all many-subband systems this scattering is mainly effective through the intrasubband scattering (due to the larger matrix element). In this case there is only one relevant final state available, i.e. $k_x' = -k_x$. If the scattering rate is sufficiently high, the effect of this interaction will be to balance the number of carriers in k_x and $-k_x$ and doing so will drastically reduce the drift velocity when an external electric field is applied. On the other hand, the coulomb interaction is strongly dependent on q_x and we can expect it to decrease strongly for large values of q_x, i.e. for large values of k_x. When an intersubband scattering takes place, we have two different final states and the scattering probability will favor the one which involves the smaller change in momentum. So, when an electric field is applied and we have a population with a given (say positive) average momentum, the preferred scattering will be the forward one and the reduction in the average velocity of the system will not be as dramatic as for the intrasubband scattering. Nevertheless, due to the divergent density of states at the bottom of each subband, most of the scattering will take place from an high energy states in one subband to a low energy states (near to the bottom of the final subband) in higher energy subband. This will result in an almost zero final velocity for the carrier.

Impurities, both inside the wire and in the confining barriers, are screened by the free carriers, as the interaction with these impurities is elastic we can introduce a screening model based on the static limit approximation. In this case the total scattering rate is simply obtained substituting the bare matrix element with the screened one. As a first approximation, this can be done with the substitution:

$$|H(q_x)| \to \frac{|H(q_x)|}{|\varepsilon(q_x)|} ,$$

where $\varepsilon(q_x)$ is the dielectric matrix obtained in the multisubband RPA approximation.

III. RESULTS AND CONCLUSION

We have investigated the effect of this interaction by varying the electric field, the lattice temperature and the doping concentration from 10^5 to 10^6 cm^{-1}. We also consider both remote impurities (in the AlGaAs layer) and uniform bulk doping. Two interesting effects are observed: At low temperature, and in particular at small electric field, most of the carriers occupy the bottom states in the band where the scattering rate is very high. Both the transient overshoot and the stationary value of the drift velocity are shown in Fig. 1 (a) and (b) for a 300 Å wide quantum wire and a doping concentration of 10^6 cm^{-1}. Here 12 subbands are included in the simulation, although only the first four are significantly populated for the fields considered. We can see that the drift veloci-

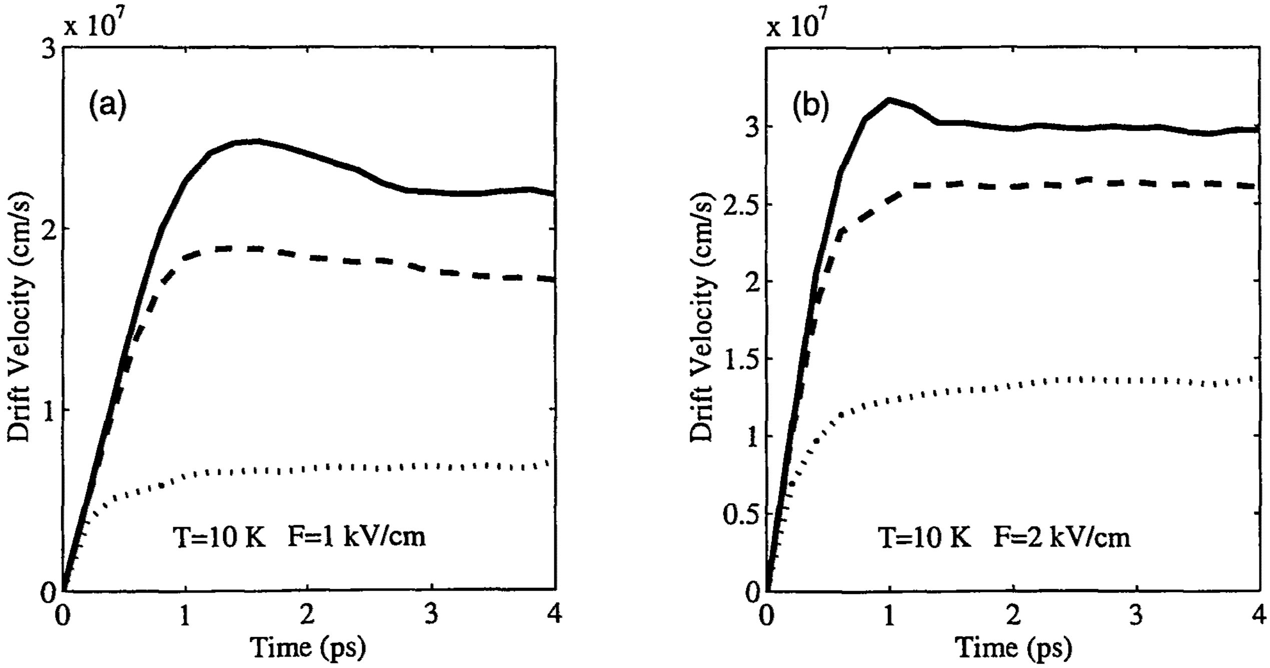

Fig. 1. Drift velocity for a wire without impurities (solid line), with remote (dashed line) and bulk (dotted line) impurities (10^6 cm^{-1}).

ty is strongly reduced by impurities in the wire (dotted line) and remote impurities (dashed line) play an important role as well (the solid line represent an ideal system with no impurities).

In Fig. 2 we plot the room temperature transient velocity under the same conditions. In this case, the remote impurities do not affect the drift velocity at all and even the effect played by the bulk impurities is strongly reduced. This is mainly due to the fact that at room temperature, most of the carriers are in higher energy states where the scattering rate is significantly smaller.

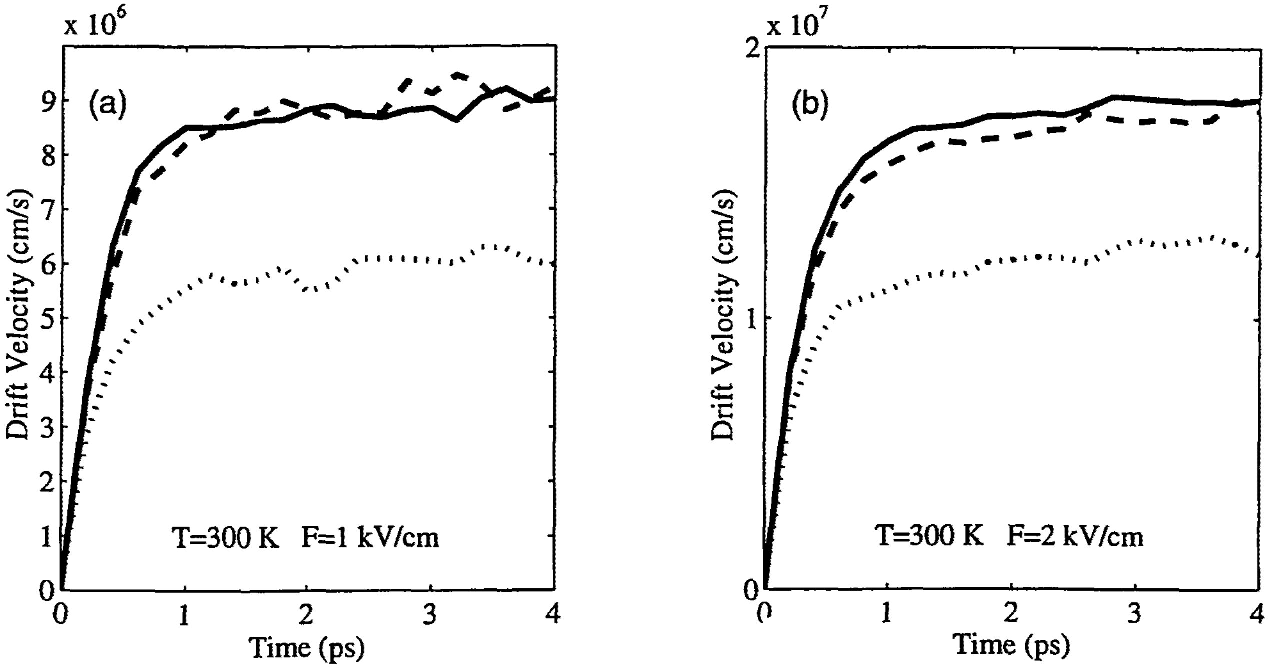

Fig. 2. Drift velocity for a wire without impurities (solid line), with remote (dashed line) and bulk (dotted line) impurities (10^6 cm^{-1}).

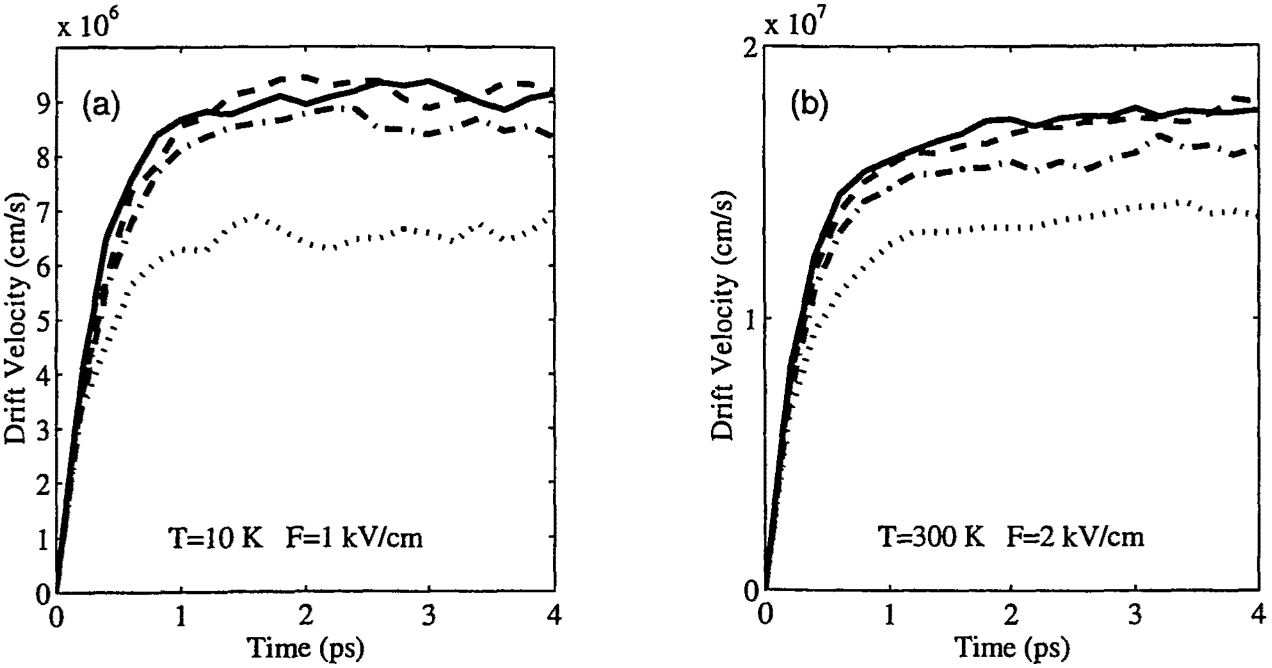

Fig. 3. Drift velocity for a wire without impurities (solid line), with remote (dashed line) and bulk (dotted line) impurities (5×10^5 cm^{-1}). The dash-dotted line represents a system with a bulk doping of 10^5 cm^{-1}.

Fig. 3 shows the same results but with a doping concentration of 5×10^5 cm^{-1}. As in the previous case, the effect of remote impurity is totally negligible and, as expected, the reduction of the drift velocity caused by bulk impurity is smaller. In the same figure the dash-dot line represents a system with a bulk doping of 10^5 cm^{-1}. Even with this low doping the drift velocity is slightly reduced.

In conclusion, we have presented a Monte Carlo investigation of impurity scattering in multi-subband quantum wires. Our results show that remote impurity do not affect significantly the transport properties of the system while direct doping in the wire can reduce the drift velocity significantly. In both cases the effect is weaker at room temperature than at low ones.

IIII. REFERENCES

[1] See e.g. *Nanostructure Physics and Fabrication*, edited by M. A. Reed and P. Kirk, Academic Press, Boston (1989).

[2] T. Demel, D. Heitmann, P. Granbow, and K. Ploog, Phys. Rev. B **38**, 12732 (1988).

[3] see e.g. U. Bockelmann and G. Bastard, Phys. Rev. B **42**, 8947 (1990), and references therein.

[4] see e.g. P. A. Knipp and T. L. Reinecke, Phys. Rev. B **48** 5700 (1993), and references therein.

[5] S. Briggs and J. L. Leburton, Phys. Rev. B **38**, 8163 (1988).

[6] K. W. Kim, M. A. Stroscio, A. Bhatt, R. Mickevicius, and V. V. Mitin, J. Appl. Phys. **70**, 319 (1991).

[7] L. Rota, F. Rossi, S. M. Goodnick, P. Lugli, E. Molinari, and W. Porod, Phys. Rev. B **47**, 1632 (1993).

[8] C. Jacoboni and P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulation* (Springer-Verlag, Berlin, 1989), and references therein.