Low-temperature electron mobilities due to ionized-impurity scattering in multisubband two-dimensional semiconductor systems

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We present a theoretical and experimental study on the low-temperature electron mobilities due to ionized impurity scattering in a multisubband quasi-two-dimensional semiconductor system. The scattering rate is obtained from the solution the Lippmann-Schwinger equation in momentum space and the screening is considered within the random-phase approximation. A quantitative agreement is reached between the theoretical and experimental results for both the quantum and transport mobilities.

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The electron mobility in two-dimensional (2D) semiconductor systems has been studied extensively. At low temperatures, the mobility in most 2D systems is dominated by ionized impurity scattering. Surprisingly, the seemingly simple impurity scattering mechanism is not fully understood yet. Although the basic physics is clear, there are theoretical details which are difficult to calculate and problematic to test against experimental data. A quantitative agreement between the experimental measured electron mobilities and theoretical calculations is still lack. In the regime where the ionized impurity scattering dominates, the electron mobility is sensitive to several factors, such as the Fermi velocity, the overlap between electrons and impurities, the screening of the electron gas and intersubband coupling through dielectric matrix, as well as the wave vector dependence of the screening potential. Other factors also affect the electron transport such as multiple scattering and weak-localization effects. In highly doped samples, spatial correlation among the impurities can also play roles. To confirm the contribution of the different effects, a quantitative agreement of theoretical calculations with experiments is of particular importance to examine the validity of the theoretical model and to understand correctly the scattering mechanism.

In a previous work, we studied in detail the electron transport mobility and quantum mobility due to impurity scattering in multisubband quasi-2D systems at low temperatures and showed that the intersubband coupling plays an essential role on the screening and transport properties.[1,2] The electron transport and quantum mobilities are determined from the different scattering times connected to the average time between the scattering events. The quantum lifetime (or the single particle relaxation time) is the average elastic scattering time. On the other hand, in order to obtain the transport lifetime (or the momentum relaxation time), every scattering event is averaged over its projection of the outgoing wave vector on the incident direction. In comparison with the experimental results, the calculated quantum mobility was in good agreement with the experimental results in the system with up to four occupied subbands,[3] but the calculated transport mobility was about two times larger than the experimental results even for the lowest subband. In fact, this difference has existed since the very earlier work about the transport properties in 2D systems.[4–6] The discrepancy between calculated transport mobility due to impurity scattering and the experimental results at low temperatures is usually attributed to other scattering mechanism such as interface roughness. However, with improvement of sample quality of the quantum well structures with almost perfect interfaces in GaAs/AlGaAs heterostructures, this discrepancy still remains. In the present work, we are interested in the ionized impurity scattering dominated electron mobilities. We study the Q2D system of δ-doping layers where no interfaces are present, the low-temperature mobility is purely determined by ionized impurity scattering. On the other hand, Zhang and Singh studied the electron transport in AlGaN/GaN heterostructures. They found that even small amount of interface roughness has very strong effect on the 2D electron gas properties. Low-lying electronic states are strongly localized and transport through these states is described by phonon-assisted hopping.[8]

Why is the quantum mobility in quantitative agreement with the experimental results but the transport mobility is not? This leads to several speculations. First, does the solution of the Boltzmann equation within the relaxation time approximation yield correctly the transport mobility? This question arises because the quantum mobility is obtained directly from the scattering rate while the transport mobility is calculated from the Boltzmann equation within the relaxation time approximation. A possible factor to reduce the transport mobility is the weak-localization effect which the Boltzmann equation is incapable to deal with. However, previous study[2] indicated that the weak-localization effect leads to a very small correction only. Second, is the RPA theory capable to describe correctly the screening effects in the electron-impurity scattering events? It is well known that the RPA screening violates the Friedel sum rule for an interacting electron gas and yields negative electronic compressibility.[7] The reliability of the RPA theory in the impurity scattering process is still an open question. Third, is the Born approximation (BA) valid to describe the scattering events? Although the BA is widely used due to its simplicity to calculate the scattering rate, one knows it is not valid in many

cases. Sahu and Patnaik[10] claimed that they examined the condition of validity of BA in coupled double quantum well structure and found that it is satisfied in their systems. However, their calculations neither went beyond the BA nor compared with experimental results. Other factors such as impurity correlations in highly doped systems could also affect the transport mobility, but they only slightly enhance the electron mobility.[11] Multiple scattering could reduce the transport mobility,[12] but it also reduces the quantum mobility which was not expected. Considering previous theoretical studies and experimental results, we believe that the effects of impurity correlation and multiple scattering are not dominant in the present problem.

In this work, we study both the transport and quantum mobilities in multisubband Q2D systems. In the calculation, we obtain the impurity scattering rate from the numerical solution of the Lippmann-Schwinger (LS) equation. To do this, we solve the multisubband LS equation in full 2D k space within the discrete momentum representation.[13] This allows us to start with the scattering matrix within the BA. On the other hand, the screening is considered within the RPA because (i) the screening is basically one-particle property, (ii) more sophisticated screening theory STLS including exchange and correlation effects yielded almost the same impurity scattering rate in 3D systems,[9] and (iii) quantitative agreement on the quantum mobility strengthens our confidence on the RPA screening potential.

The calculations are applied to the δ-doped semiconductor systems and compared to our experimental results. The eigenenergy and wave function are obtained by the self-consistent solution of the coupled Schrödinger and Poisson equations and the mobilities are calculated for each subband as a function of the total electron density. Notice that in all our calculations no fitting or adjustable parameters are used. Our main result in this work is that we simultaneously obtain the quantitative agreement between the theoretical and experimental results for both the quantum and transport mobilities. The long-standing puzzle about the electron transport mobility in 2D systems may have a simple explanation. Such a quantitative agreement also confirms the validity of RPA screening for the impurity scattering problem in 2D electron transport.

A full application of the LS equation in momentum space to the problem of electron scattering on an atomic and molecular target can be found in the literature (see, for example, Refs. 14–18). The theoretical procedure consists basically in carrying out the partial-wave expansion of the LS equation and then numerically solving a set of coupled one-dimensional LS integral equations in momentum space. Though this procedure is applicable in the present problem, it is not recommended once the calculation of the 2D partial-wave projection of the potential matrix elements requires the knowledge of the interaction potential $u_{n,n'}$ in the real 3D space. However, the LS equation can be numerically solved using the discrete momentum representation (DMR) proposed by Polasek *et al.*[13] and applied to the calculations of the e^--H_2 (Ref. 13) and e^--CH_4 (Ref. 19) elastic scattering cross sections. In this method, the transition matrix is written in the full 3D momentum space using numerical quadrature

$$\langle \vec{k}_f|T_{n,n'}|\vec{k}_i\rangle = \langle \vec{k}_f|u_{n,n'}|\vec{k}_i\rangle + \int d^3\vec{k}\frac{\langle \vec{k}_f|u_{n,n'}|\vec{k}\rangle\langle \vec{k}|T_{n',n}|\vec{k}_i\rangle}{k_i^2 - k^2 + i\epsilon}. \tag{1}$$

Here, we extend the DMR method to multisubband scattering problem in Q2D system. We also notice that for a Q2D system of symmetrical confinement potential with two occupied subbands, the intersubband scattering potential vanishes. In this case, we need to carry out the diagonal transition matrix elements only in the LS equation so that the solutions can be obtained in an independent way for each conduction channel n. For the system with more than two occupied subbands, the intersubband interaction is finite between two subbands of the same parity. In this case, we treat the off-diagonal matrix elements within the BA for simplicity because the intersubband scattering is not dominant. We express the LS equation in polar coordinates $\vec{k} \equiv (k, \theta)$ as

$$\langle \vec{k}_f|T_n|\vec{k}_i\rangle = \langle \vec{k}_f|u_n|\vec{k}_i\rangle + \int_0^\infty kdk\frac{f_n(\vec{k}_f,\vec{k}_i;k)}{k_i^2 - k^2 + i\epsilon} \tag{2}$$

with

$$f_n(\vec{k}_f,\vec{k}_i;k) = \int_0^\pi d\theta\langle \vec{k}_f,\vec{k}_i|u_n|k,\theta\rangle\langle k,\theta|T_n|\vec{k}_i\rangle, \tag{3}$$

where $|k_i| = k_{F_n} = \sqrt{2E_{F_n}}$. In Eq. (2), the first term on the right-hand side is the first BA matrix element. We solve the above equation through an integral discretization by an appropriated quadrature set. In the numerical calculations, we first change the integration interval $(0,\infty)$ for the radial part to an interval $(-1,1)$ through the relation $x=(k-k_i)/(k+k_i)$ and this interval is divided as $2N$ points of a Gauss-Legendre integration quadrature, while the angular part is equally divided into l points in the $0 \leqslant \theta \leqslant \pi$ interval. This quadrature application permits us to write the LS equation in matrix form

$$\tilde{T}_n = \tilde{U}_n + \tilde{U}_n\tilde{G}_n^{(0)}\tilde{T}_n, \tag{4}$$

where $G_n^{(0)}$ is the free particle Green function in the 2D momentum space.[20] The transition matrix $\tilde{T}$ can be obtained through a matrix inversion operation

$$\tilde{T}_n = (\tilde{1} - \tilde{U}_n\tilde{G}_{0,n})^{-1}\tilde{U}_n. \tag{5}$$

The scattering rate is given by $\Gamma_n(k_{F_n},\theta) = (m^*/\pi\hbar^3)|T_n(k_{F_n},\theta)|^2$ from which we can obtain the electron mobilities.[1]

Starting from the electron-impurity scattering rates within the BA, we obtain here the mobilities from the solution of the LS equation within the DMR in the Si δ-doped GaAs system. The δ-doping layer is 20-Å thick and all the impurities are ionized. The background acceptor density is taken as 10^{14} cm^{-3}. In Figs. 1(a) and 1(b) we plot the ratio of the scattering rates obtained within the DMR and the BA as a function of the scattering angle for the conduction electrons in the first and the second subbands, respectively. The calculated results are presented for different electron densities

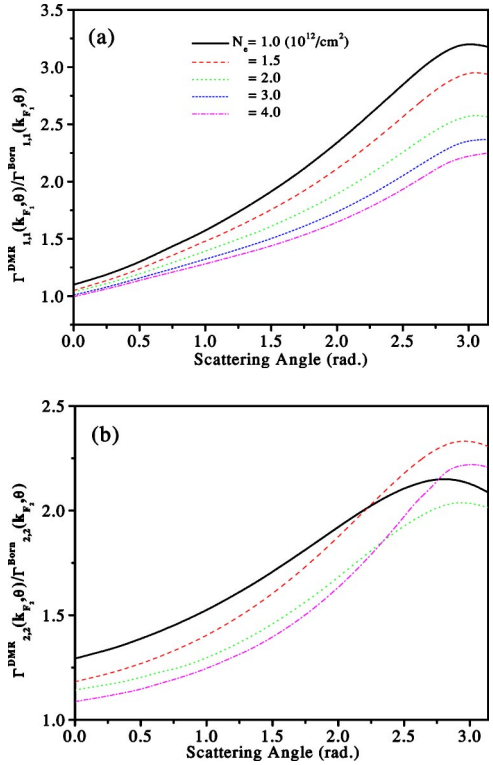

FIG. 1. The ratio of the scattering rates obtained within the LS equation and the Born approximation for conduction electrons in (a) the first and (b) the second subbands for the δ-doped systems with different densities.

(Fermi energies) in the system. This ratio is larger than 1 as expected and it increases with increasing the scattering angle because the BA underestimates the scattering especially for large-angle scattering.

Figure 2 shows the theoretical and experimental results of (a) the quantum and (b) transport mobilities of the electrons in the first and second subbands as a function of total electron density in the Si δ-doped GaAs systems. In general, both the quantum and the transport mobilities are reduced with the rigorous treatment of the scattering rate, but the transport mobility becomes significantly smaller in comparison to that within the BA. Quantitatively, the quantum mobility is still in good agreement with the experimental results. At the same time, the transport mobility becomes very close to the measured results. For the first subband, they are in excellent agreement. For the second subband, though they become close to each other, full quantitative agreement is not achieved yet. We believe the experimental results for the second subband could be of a large error because they are obtained with a two-subband model where there are actually three occupied subbands for $N_e > 1.62 \times 10^{12}$ cm^{-2}.

The experimental measurements of the electron mobility in each subband are not a simple task in a multisubband system.[21] The subband quantum mobility, defined by the quantum lifetime of the electrons in each subband, is obtained with a relatively good precision by analysis of the Shubnikov–de Haas oscillations of the longitudinal magnetoresistance. The error of the measured quantum mobility is in order of 15% for lower subbands. However, the transport

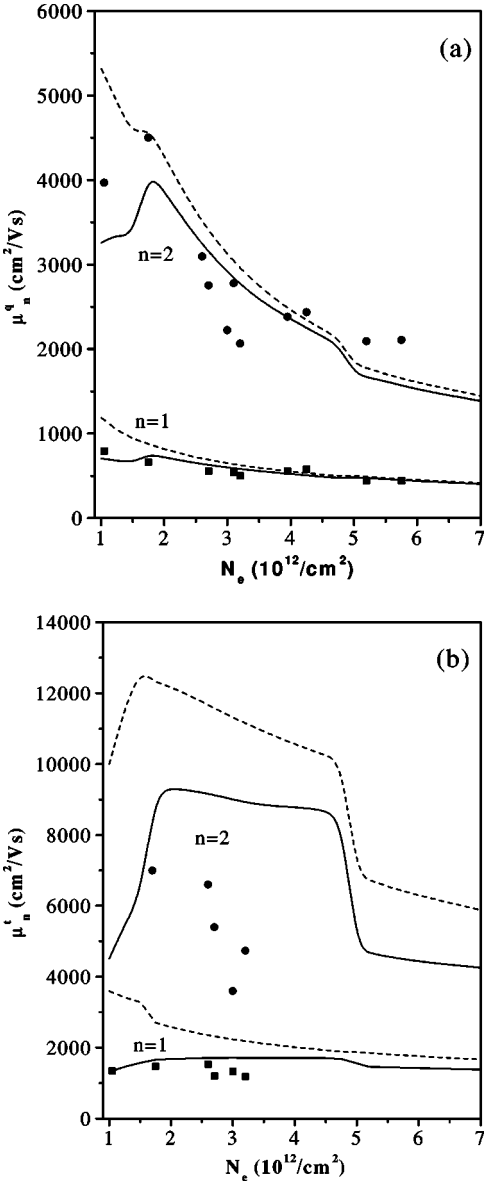

FIG. 2. (a) The quantum and (b) the transport mobilities for the first ($n=1$) and second ($n=2$) subbands in the δ-doped system. The solid and dashed curves are obtained within the LS equation and the Born approximation, respectively. The experimental mobilities are indicated by the symbols.

mobility (which determines the electrical conductivity) of an individual subband is difficult to be determined from the magnetoresistance measurement. They are estimated by the so-called mobility spectrum technique which is considered the best way one can do. Even though, this method works reasonably well just for the system of two occupied subbands with weak intersubband scattering, actually, in most cases, we can obtain reliable results for the lowest subband only. Furthermore, the ratio of the transport mobility to the quantum mobility is an interesting parameter. For δ-doping layers, the experimental value is about 2 to 3 which is in agreement with the present theoretical results. It increases with increasing electron density.

To understand better the impurity scattering problem, we calculate the screened impurity potential in real space due to

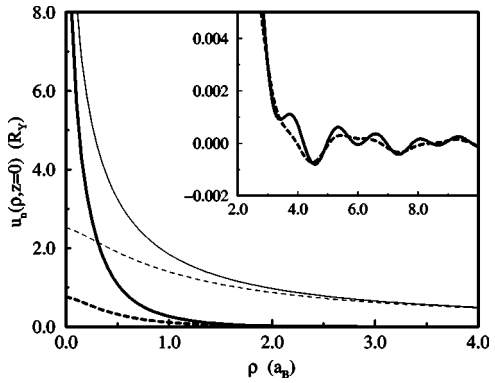

FIG. 3. The bare (thin curves) and screened (thick curves) impurity potential at the $z=0$ plane in the real space for electrons in the first (solid curves) and the second (dashed curves) subbands. $N_e=10^{12}$ cm^{-2}, $R_y=5.48$ meV, $a_B=99.8$ Å, $E_{F1}=25.50$ meV, and $E_{F2}=4.18$ meV. The inset shows the Friedel oscillations.

a multisubband Q2D electron gas.[22] We obtain the electron-impurity interaction potential $u_n(\rho,z)$ within the RPA for an electron at $\vec{r}=(\vec{\rho},z)$ in subband n (the impurity is at $\vec{r}=0$ and center of the δ layer is $z=0$). Figure 3 shows the bare and screened potential in real space at the $z=0$ plane in the δ-doped system. The screening reduces substantially the impurity potential which is significant only for $r<a_B$. Therefore, the spatial impurity correlation only enhances slightly the electron mobility.[11] The BA is failed for the transport mobility because the large-angle scattering occurs for short-distance scattering. We show that the screening theory within the RPA is good enough for the electron-impurity scattering in doped Q2D semiconductor systems even with multisubband occupation.

In conclusion, we have studied both the electron transport and quantum mobilities in a consistent fashion in a Q2D semiconductor system. We have achieved a quantitative agreement between the theoretical and the experimental results both for the quantum and the transport mobilities. We apply the method of the discrete momentum representation for the Lippmann-Schwinger equation to study the multisubband ionized impurity scattering and the electron transport in Q2D systems. Our results show that is the widely used BA responsible for previous higher theoretical transport mobility. On the other hand, our quantitative agreement between the theory and experiment for both mobilities confirms that the screening within the RPA for the ionized impurity scattering describes the multisubband electron transport in Q2D systems reasonably well.

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