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Short-range disorder effects on electronic transport in two-dimensional semiconductor structures

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We study theoretically the relative importance of short-range disorder in determining the low-temperature two-dimensional (2D) mobility in GaAs-based structures with respect to Coulomb disorder, which is known to be the dominant disorder in semiconductor systems. We give results for unscreened and screened short-range disorder effects on 2D mobility in quantum wells and heterostructures, comparing with the results for Coulomb disorder and finding that the asymptotic high-density mobility is always limited by short-range disorder which, in general, becomes effectively stronger with increasing "carrier density", in contrast to Coulomb disorder. We also predict an intriguing reentrant metal-insulator transition at very high carrier densities in Si metal-oxide-semiconductor field-effect transistors driven by the short-range disorder associated with surface-roughness scattering.

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One of the most spectacular applied physics and electronic materials advances of the past 40 years has been the 2000-fold enhancement of the low-temperature carrier mobility in molecular beam epitaxy (MBE)-grown GaAs-based two-dimensional (2D) semiconductor structures. Between 1978, when the modulation doping technique was introduced by Störmer *et al*. [1] in 2D *n*-GaAs-AlGaAs heterostructures, and now (i.e., 2014), the electronic mobility (μ) at low temperatures (below the Bloch-Grüneisen temperature scale, where phonons are unimportant [2]) has increased in 2D GaAs systems from $\mu \approx 2 \times 10^4$ cm^2/V s to $\mu \approx 4 \times 10^7$ cm^2/V s [3] due to the steady improvement in purity, growth, fabrication, and processing techniques of individual 2D GaAs samples. As an aside, it may be pointed out that this increase in low-temperature mobility in 2D GaAs structures is comparable in magnitude to the much better known Moore's law exponential increase in the room-temperature microprocessor speed in complementary metal-oxide semiconductor (CMOS) devices achieved over the same time scale, although the qualitative origins of the two enhancements are very different [better molecular beam epitaxy (MBE) growth and improved modulation doping for individual 2D *n*-GaAs structures whereas better packaging and miniaturization for Si microprocessors].

In this Rapid Communication, we study theoretically the harmful effects of short-range disorder scattering in limiting the low-temperature electronic mobility in 2D GaAs structures, contrasting short-range disorder scattering with the corresponding long-range Coulomb disorder scattering arising from quenched charged impurities, which has been extensively studied in the literature [4,5]. It is well known that Coulomb disorder arising from unintentional charged impurities in the background and from the intentional dopants needed in order to produce free carriers in semiconductors is the main mobility-limiting scattering mechanism in high-mobility 2D GaAs structures. However, at higher carrier densities, where Coulomb disorder is strongly screened out, other weaker and short-ranged scattering mechanisms arising from alloy disorder, interface roughness, neutral impurities, and defects could play a quantitative role in determining the 2D mobility in high-mobility 2D GaAs systems. Theoretically studying the quantitative effect of such short-range disorder scattering is the goal of this work.

Our theory uses the $T = 0$ Boltzmann transport equation for calculating the carrier mobility (μ) limited by individual scattering mechanisms by directly calculating the relevant transport relaxation or scattering time (τ), with the mobility being defined as $\mu = e\tau/m$ and the conductivity σ given by $\sigma = ne\mu$, where n is the 2D carrier density (and m the carrier effective mass). Within the leading-order Born approximation the disorder-induced scattering rate τ^{-1} is given (at $T = 0$) by [6,7]

$$\frac{1}{\tau_i(k)} = \frac{2\pi}{\hbar}\int \frac{d^2k'}{(2\pi)^2}\int_{-\infty}^{\infty} dz N_i(z)\frac{|V_i(q,z)|^2}{\epsilon(q)^2} \times (1-\cos\theta)\delta(E_k - E_{k'}). \quad (1)$$

Here i denotes the ith type of disorder characterized by a random distribution of scattering centers with density $N_i(z)$ along the z direction normal to the 2D layer, with V_i being the bare impurity potential and $\epsilon(q)$ the static random-phase approximation (RPA) dielectric screening function for the 2D carrier system. If screening is irrelevant as it is for most short-range disorder, we take $\epsilon(q) = 1$. Also, $E_k = \hbar^2k^2/2m$ is the 2D carrier energy. The functions V_i, ϵ, etc., are to be calculated in the appropriate basis of the quasi-2D quantized confinement wave function (along the z direction) of the 2D semiconductor structure so that they are really matrix elements in the appropriate ground subband of the 2D system. For Coulomb disorder, $V_i(q,z) = (2\pi e^2 Z_i/\kappa q)e^{-qz}$, where κ is the background lattice dielectric constant and Z_i is the impurity charge strength of the charged center producing the disorder. For short-range disorder, we assume, with no loss of generality, $V_i \equiv V_0\delta(\mathbf{r} - \mathbf{r}_i)\delta(z - z_i)$, an uncorrelated delta-function white noise disorder characterized by a potential strength V_0 (as well as an impurity density N_i). It is then straightforward to calculate the short-range scattering rate,

$$\frac{1}{\tau(k)} = mN_iV_0^2C\int_0^2 \frac{dx}{\sqrt{4-x^2}}\frac{x^2}{\epsilon(kx)^2}, \quad (2)$$

where $C = \int |\xi_0(z)|^4 dz$, with $\xi_0(z)$ being the ground-state quasi-2D confining wave function defining the quantum bound state of the 2D system along the z direction, i.e., the total single-particle ground-state wave function is given by

$\psi_0(\mathbf{r},z) = \xi_0(z)e^{i\mathbf{k}\cdot\mathbf{r}}$, where $\mathbf{r}$ and $\mathbf{k}$ are the 2D position and wave vector, respectively.

If screening is neglected and the 2D system is approximated to be an idealized zero-thickness layer, then $\epsilon = 1$ and $C = 1$, so that the scattering rate $[\tau(k)]^{-1} = mN_iV_0^2$ is a constant determined only by the strength of the short-range disorder (and carrier effective mass), becoming completely independent of 2D wave vector and carrier density. (In practice, there might be some carrier density dependence even in the absence of screening because of the quasi-2D form factor associated with the confinement wave function.) If it is appropriate to screen the short-range disorder using the static RPA dielectric function $\epsilon(q) = 1 + q_{TF}/q$, where q_{TF} is the 2D screening wave vector, Eq. (2) gives

$$\frac{1}{\tau(k)} = mN_iV_0^2Ck^2\int_0^2 \frac{dx}{\sqrt{4-x^2}}\frac{x^4}{(kx+q_{TF})^2}. \qquad (3)$$

Putting $k = k_F \propto \sqrt{n}$ as appropriate at $T = 0$, Eq. (3) implies that the 2D mobility μ $[\propto\tau(k_F)]$ limited by screened short-range disorder has the following high- and low-density behavior (ignoring any density dependence arising from the confinement wave-function effects, i.e., in the strict 2D limit)

$$\begin{aligned} \mu &\sim n^0, \quad q_{TF} \ll 2k_F, \\ &\sim n^{-1}, \quad q_{TF} \gg 2k_F. \end{aligned} \qquad (4)$$

Thus, the high-density limit of the screened situation is the same as the unscreened case of no density dependence (since $q_{TF} \ll 2k_F$ in the high-density limit), but the low-density (and strongly screened $q_{TF} \gg 2k_F$) situation produces the somewhat counterintuitive $\mu \sim n^{-1}$ dependence where increasing (decreasing) 2D carrier density suppresses (enhances) the 2D mobility constrained by short-range disorder scattering. By contrast, the Coulomb disorder limited mobility behaves as $\mu \sim n^{\alpha(n)}$, with $\alpha(n \to 0) \sim 0$ and $\alpha(n \to \infty) \sim 1$ or $3/2$ depending respectively on whether the charged impurities are near or far from the 2D layer [5]. Thus, Coulomb disorder limited 2D mobility always increases with increasing 2D carrier density whereas the short-range disorder limited 2D mobility is either a constant independent of density or decreases with increasing density. This immediately implies that short-range disorder becomes increasingly more important at higher carrier densities where Coulomb disorder is increasingly suppressed. (In fact, similar transport behavior occurs also in graphene [7], where the low- to intermediate-density mobility is a constant because of Coulomb disorder whereas the high-density mobility decreases with increasing carrier density because of short-range scattering.) Thus, the low-temperature high-density maximum mobility of all 2D systems is eventually always limited by short-range scattering since the Coulomb disorder limited scattering is strongly and monotonically suppressed with increasing density. This behavior is well known in 2D Si metal-oxide-semiconductor field-effect transistors (MOSFETs) [6] and in graphene [8,9], but is true for 2D GaAs systems also where the mobility must saturate (or even decrease) at high enough carrier density because any existing short-range disorder (no matter how small) arising from alloy disorder or interface roughness or neutral defects would eventually dominate the high-density mobility once the Coulomb scattering effects have become negligible. (The 2D Coulomb disorder case has recently been discussed in depth by us elsewhere [4,5].)

We note that the fact that the low- (high)-density regime is more strongly (weakly) screened than the high- (low)-density regime follows simply from the Fermi wave vector k_F going as $n^{1/2}$ in 2D versus the screening wave vector q_{TF} going as a constant—the same situation applies in three-dimensional (3D) systems, too, where $k_F \sim n^{1/3}$ and $q_{TF} \sim n^{1/6}$. This is simply a universal feature of the dimensionless quantum screening parameter $q_{TF}/2k_F$ increasing with decreasing carrier density in a quantum degenerate electron gas—obviously, the absolute magnitude of screening (i.e., q_{TF} itself) always increases with increasing density both in quantum and classical situations. While any long-range Coulomb disorder (arising from random charged impurity scattering) must always be screened, the short-range disorder may or may not always be screened depending on its physical origin—for example, the short-range disorder arising from interface roughness (atomic defects or vacancies) should typically be screened (unscreened).

We now present our detailed numerical results for 2D mobility limited by short-range scattering, comparing and contrasting with the corresponding Coulomb disorder situation. Our numerical results (all at $T = 0$) include full effects of the appropriate quasi-2D confinement wave function in our calculations, both for GaAs quantum wells [where the well width a determines $\xi_0(z)$] and heterostructures [where the ground-state confinement wave function $\xi_0(z)$ depends explicitly on the carrier density n through the self-consistency effect [6,10], thus providing an additional density dependence of the mobility]. Our use of the Born approximation in the Boltzmann transport theory is justified by the high carrier density regime of our interest, and is also borne out by the extensive success of the Born approximation in calculating 2D semiconductor transport properties over the past 40 years, both for long-range Coulomb disorder and short-range interface roughness disorder. [6] We mention also that the parameters used for our transport calculations are realistic numbers for Si MOS structures [6], but not for GaAs-based 2D systems, where the interface roughness scattering is much weaker than in Si MOSFETs since the GaAs-AlGaAs interface has very little roughness, with GaAs and AlGaAs being almost lattice matched. The other differences between Si and GaAs systems are the different effective masses, background dielectric constants, and lower impurity disorder in GaAs.

In Figs. 1–3 we show respectively our numerical results for the mobility (μ) as a function of carrier density (n) in GaAs-AlGaAs heterostructures (Fig. 1) and GaAs-AlGaAs quantum wells (Figs. 2 and 3). In each case, $\mu(n)$ as well as the density scaling exponent $\alpha(n) \equiv d\ln\mu/d\ln n$ of mobility [5], i.e., $\mu \sim n^{\alpha}$, are both shown for several different models of long- and short-range disorder scattering: unscreened and screened Coulomb disorder and unscreened and screened neutral short-range disorder. In Figs. 1 (heterostructure) and 2 (quantum well), the impurities are located inside the 2D electron layer whereas in Fig. 3 (quantum well) the impurities are located at the interface. The absolute magnitudes of the mobilities are not particularly relevant since the impurity densities (or the scattering strength) are not known in general, but the relative

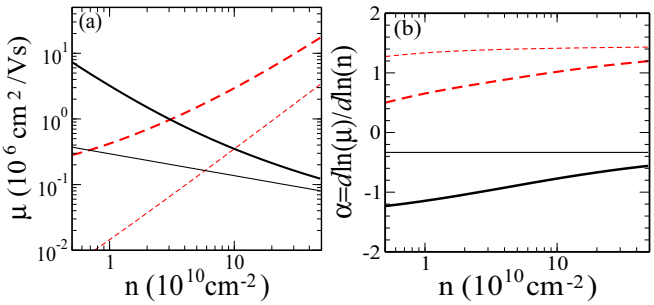

FIG. 1. (Color online) Calculated (a) mobility and (b) exponent as a function of density for GaAs-AlGaAs heterostructures. The solid (dashed) lines show the results calculated with short-range (long-range) disorder scattering. The thick (thin) lines represents the results for screened (unscreened) disorder. All impurities are located inside the 2D electron layer.

variations in the mobility as a function of density for various scattering mechanisms provide a meaningful comparison. We adjusted the various unknown impurity parameters (e.g., N_i for Coulomb disorder and $N_i V_0^2$ for short-ranged disorder) so that all the results for different scattering mechanisms can be fitted within the same figure. It is easy to obtain the mobility limited by arbitrary scattering strength (i.e., different values of N_i and/or V_0^2) simply by appropriately scaling our results shown in Figs. 1–3, remembering that $\mu^{-1} \propto N_i$ (or $N_i V_0^2$).

The most important qualitative results of Figs. 1–3 are the following: (i) The mobility often, but not always, could decrease with increasing density for short-range disorder scattering; (ii) the high-density mobility is always dominated by short-range disorder; (iii) a consequence of the last statement is that at sufficiently high density $\alpha(n)$, where $\mu(n) \sim n^{\alpha}$, will either become zero or become negative; (iv) the detailed quantitative aspects of short-range disorder effect on the mobility would depend on many (unknown) microscopic details such as the location of the disorder (at the interface or in the layer), screened or not, quantum well or heterostructure; (v) the 2D mobility, when limited by short-range disorder in the channel, has an exponent $-2 \lesssim \alpha \lesssim 0$, which is qualitatively different from the exponent α limited by Coulomb disorder

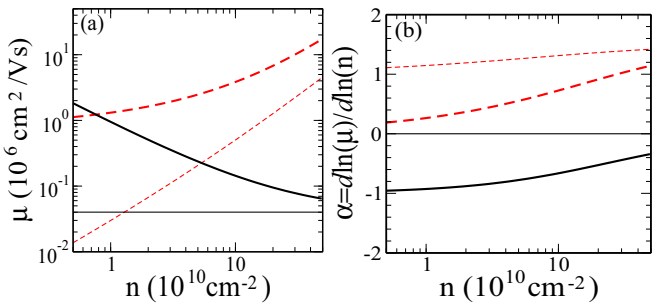

FIG. 2. (Color online) Calculated (a) mobility and (b) exponent as a function of density for GaAs-AlGaAs quantum wells with well width $a = 200$ Å. The solid (dashed) lines show the results calculated with short-range (long-range) disorder scattering. The thick (thin) lines represents the results for screened (unscreened) disorder. All impurities are located inside the 2D quantum well.

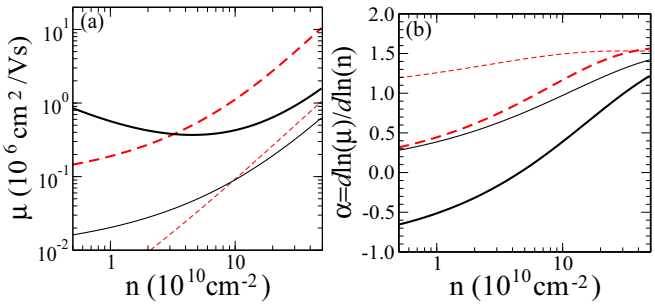

FIG. 3. (Color online) The same as Fig. 2, but the impurities are located at the interface.

($\alpha > 0.5$)—whether α is actually zero or negative depends on whether the short-range disorder is screened or not; and (vi) the mobility decreases linearly with N_i, and thus it decreases linearly with the number of Al atoms (i.e., Al density) in the channel, assuming that the mobility is limited by alloy disorder scattering [11].

We note that it is straightforward to derive the following dependence of mobility limited by unscreened short-range disorder on the quasi-2D form factor arising from the wave-function confinement effect:

$$\frac{1}{\tau_k} = m N_i V_0^2 \begin{cases} 3b/16, & \text{heterostructure}, \\ 3/2a, & \text{quantum well}, \end{cases} \tag{5}$$

where a is the quantum well width and b is the variational parameter defining $\xi_0(z)$ ($\sim z e^{-bz/2}$), which is given by $b \propto n^{1/3}$ in the simple Stern-Howard variational approximation [6]. In general, $b \propto n^{1/3}$ and $a \propto n^0$, and thus $\mu \sim n^{-1/3}$ (heterostructure) and $\mu \sim n^0$ (quantum well) for the unscreened short-range disorder. In the presence of screening, an extra factor of $1/k_F^2$ comes in [see Eq. (3)] so that we get $\mu \sim n^{-4/3}$ (heterostructure) and $\mu \sim n^{-1}$ (quantum well) in the $q_{TF} \gg 2k_F$ limit of screened short-range disorder. For $q_{TF} \ll 2k_F$, the screening effect disappears, as discussed earlier.

Finally, we conclude by making an intriguing prediction about a reentrant metal-insulator transition which should occur in 2D Si MOSFETs at a very high carrier densities ($>10^{13}$ cm^{-2}) driven entirely by the short-range disorder scattering associated with the surface roughness at the Si-SiO_2 interface, which is known to be the dominant high-density mobility-limiting mechanism [6]. As shown in Fig. 4, the Si MOSFET mobility $\mu(n)$ at first increases (for $n < n_m$) with increasing carrier density, reaching a maximum sample-dependent value μ_m at some characteristic sample-dependent density n_m, with $\mu(n > n_m)$ decreasing with increasing carrier density at high density [6]. The numerical results shown in Fig. 4 are easily understood based on the realistic model of just two scattering mechanisms, leading to mobilities limited by Coulomb impurities ($\mu_{\rm CI}$) and surface roughness ($\mu_{\rm SR}$) dominating at low ($n < n_m$) and high ($n > n_m$) densities, respectively,

$$\mu = \left[\mu_{\rm CI}^{-1}(n) + \mu_{\rm SR}^{-1}(n)\right]^{-1}, \tag{6}$$

with $\mu_{\rm CI}(n) \sim n^{\alpha_{\rm CI}(n)}$, where $\alpha_{\rm CI} \sim 0.4$, and $\mu_{\rm SR}(n) \sim n^{\alpha_{\rm SR}(n)}$, where $\alpha_{\rm SR} \sim -2$. From Eq. (6), we then get

$$\mu = (An^{-0.4} + Bn^2)^{-1}, \tag{7}$$

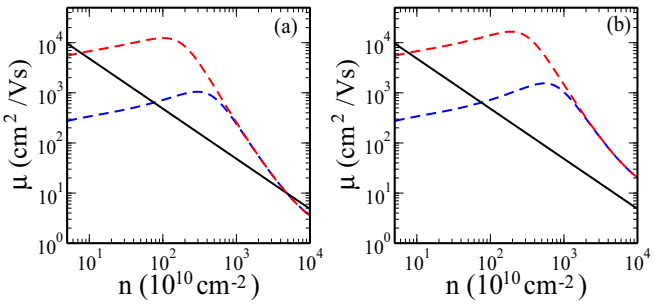

FIG. 4. (Color online) Calculated mobility in Si MOSFETs as a function of density. The solid line represents $\mu = (2e/h)(1/n)$, which is equivalent to $k_F l = 1$. The top (bottom) dashed line (in each figure) represents the mobility of a high- (low-) quality Si MOSFET (i.e., with a large or small amount of Coulomb disorder). The surface-roughness parameters, $\Delta = 10$ and 4.5 Å, are used in (a) and (b), respectively (see Ref. [6] for details). (a) and (b) correspond respectively to roughness parameters allowing (or not) a reentrant transition to a high-density insulating phase—see the text for details.

where A and B are constants (i.e., roughly independent of carrier density) which depend on the details of Coulomb disorder and surface-roughness disorder, respectively. Equation (7) implies $\mu(n \to 0) \sim n^{0.4}$ and $\mu(n \to \infty) \sim n^{-2}$, and thus $\mu(n)$ has a maximum at a disorder-dependent nonuniversal density $n_m(A,B)$ with the value $\mu_m = \mu(n_m)$. It is easy to show $n_m \approx 1.7(A/B)^{0.4} \propto 1.7(N_{\rm CI}/V_{\rm SR}^2)^{0.4}$, where $N_{\rm CI}$ and $V_{\rm SR}^2$ are the charged impurity disorder strength and surface-roughness scattering strength, respectively. Thus, n_m (μ_m) increases (decreases) with increasing charged impurity density. All of these behaviors are clearly manifest in our Fig. 4, where we show realistic numerical results for two situations with low and high values of $N_{\rm CI}$ (thus corresponding to a high-quality and a low-quality MOSFET sample, respectively) using the same surface-roughness disorder parameters. The two sets of results in Fig. 4 [i.e., Figs. 4(a) and 4(b)] correspond to using two different sets of surface-roughness material parameters at the Si-SiO_2 interface, which are in general not independently known and often inferred based on the modeling of transport measurements.

What we summarize above is known in some form in the literature on Si MOSFET transport properties [6], but now we make an observation which seems to have been overlooked in the extensive literature on MOSFETs. We note that the transport mean free path (l), $l = v_F\tau = v_F m\mu/e$, with $v_F = p_F/m = \hbar k_F/m$ being the Fermi velocity, is very small in Si MOSFETs both at low carrier density (where Coulomb scattering dominates) and at high carrier density (where short-range surface-roughness disorder dominates). It is well known that Si MOSFETs universally undergo a low-density metal-insulator transition (MIT) at a critical density n_{c1} ($<n_m$), dominated by charged impurity scattering, where the mean free path becomes short enough so that the Ioffe-Regel-Mott criterion $k_F l = 1$ is satisfied. This low-density MIT in Si MOSFETs has been studied extensively in the literature over the past 40 years [6,7,12]. What we predict here is that the Ioffe-Regel-Mott criterion may also be satisfied at high density ($n > n_m$), where very strong short-range surface-roughness scattering would eventually reduce the mobility to a low enough value (<100 cm^2/V s) so that $k_F l = 1$ would be satisfied at a second critical density n_{c2} ($>n_{c1}$) with the insulating state being reentrant for $n > n_{c2}$ (as well as for $n < n_{c1}$) and the intermediate $n_{c1} < n < n_{c2}$ density regime being metallic. We show $k_F l = 1$, which is equivalent to the $\mu = (2e/h)(1/n)$ line, in our Fig. 4 to emphasize the fact that there can, in principle, be two solutions for the integral equation $k_F l = 1$ at two densities, depending on the details of disorder. Our extensive numerical investigations with many possible realistic Si MOSFET disorder parameters show that $n_{c2} \gtrsim 10^{13}$–10^{14} cm^{-2} in general, with $n_{c2} \approx 3$–5×10^{13} cm^{-2} being the most likely value for most realistic Si MOSFET samples. By contrast, $n_{c1} \gtrsim 10^{11}$–10^{12} cm^{-2}, typically depending on the amount of Coulomb disorder in the system. Of course, it is also possible that the surface-roughness scattering is never strong enough to induce a $k_F l = 1$ condition at any carrier density, in which case there will be no reentrant transition to an insulating phase at high carrier density as shown in Fig. 4(b).

If low-temperature transport measurements are feasible in Si MOSFETs at carrier densities above 10^{13} cm^{-2}, we believe that our predicted reentrant metal-insulator transition could be observed experimentally. We emphasize, however, that the integral equation $\mu(n) = (2e/h)(1/n)$ may have zero, one [Fig. 4(b)], or two [Fig. 4(a)] solutions in general, depending on the details and the relative strengths of the applicable long- and short-range disorder in the system, given that $\mu(n) \sim n^{-2}$ for $n \to \infty$ and $\sim n^{0.4}$ for $n \to 0$. The three solutions correspond respectively to the system being always localized because of very large disorder ($k_F l < 1$ for all densities), having an insulating phase at low density $n < n_{c1}$ driven by Coulomb disorder and a metallic phase for all $n > n_{c1}$ [as in Fig. 4(b)], and the reentrant insulating case with a second insulator for $n > n_{c2}$ [as in Fig. 4(a)] driven by strong surface-roughness disorder. The first two situations are well known in the MOSFET literature, but the reentrant high-density insulating phase predicted here still needs to be reported experimentally to the best of our knowledge.

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