Use of low-temperature Hall effect to measure dopant activation: Role of electron-electron interactions

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A complete understanding of the activation of phosphorus dopants in silicon as a function of doping density is important for the fabrication of silicon transistors and devices as they scale down in size to the atomic level. Here, we present a systematic study of the low-temperature Hall effect in Si:P δ-doped layers with degenerate doping densities in the range $(\sim 0.2-2)\times 10^{14}$ cm^{-2}, from just above the transition to strong localization to the highest carrier densities achievable. Importantly, at low temperatures, we find a temperature dependent correction in the Hall coefficient consistent with that predicted by electron-electron interaction theory. This correction manifests as an apparent decrease in the carrier density determined from conventional Hall measurements of up to ~50% in low density samples and can be mistakenly interpreted as reduced dopant activation. After correcting for electron-electron interaction effects, we demonstrate that all P dopants in the Si:P δ-doped layers are electrically active for the complete range of doping densities studied.

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Over the past decade, there has been a growing interest in developing highly doped silicon due to the need to maintain a sufficient conductance of source/drain regions in nanoscale field effect transistors.[1,2] One way to achieve this is to use low-temperature molecular beam epitaxy to encapsulate a two-dimensional (2D) sheet of dopants (δ-doped layer) in silicon, thereby achieving high dopant concentrations with abrupt doping profiles.[3] A recent report has suggested that constraining high concentrations of dopants in two dimensions can strongly inhibit the formation of deactivating defects in silicon,[4] allowing full electrical activation to be achieved. Thus, a highly δ-doped system can potentially provide a significantly higher carrier density than its equivalently bulk doped counterpart. In addition, the technique of δ doping has been shown to provide a higher carrier mobility compared to bulk doping.[5]

Numerous studies have attempted to probe the limits of δ-doping carrier density.[5–8] Thus far, the highest free carrier density[5] achieved in Si-based δ-doped samples is $\sim 3\times 10^{14}$ cm^{-2}, with the lowest being $\sim 10^{13}$ cm^{-2} below which they become insulating. In the doping range of $10^{13}-10^{15}$ cm^{-2}, they are intrinsically disordered 2D conductors exhibiting typical carrier mobilities of $\sim 20-100$ cm^2 V^{-1} s^{-1}. For such layers, it is important to use a reliable method to determine the carrier density n_s. A direct determination of n_s from the analysis of Shubnikov–de Haas oscillations is not possible since it requires prohibitively large magnetic fields of 100 T or more which are not experimentally feasible. It is therefore common practice to determine n_s from either room temperature or low-temperature Hall-effect measurements. Previous studies of such low mobility δ-doped samples have observed *reduced dopant activation* either at (i) high carrier densities when measured at low temperatures, which has been attributed to the formation of defects,[9] or (ii) over a range of carrier densities when measured at room temperature, which has been attributed to the effects of carrier confinement in the potential well of the highly doped δ layer.[5]

Recently, the combination of Si:P δ doping in conjunction with scanning probe lithography has been suggested as a strategy for realizing nano- to atomic-scale dopant profiles in silicon.[10–12] To observe the effects of quantum confinement of the electrons in these atomically precise devices, they typically have to be cooled to low temperatures (e.g., 4.2 K or below) where electron-phonon interactions are quenched.[13] This is particularly the case for devices which employ lithography using scanning tunneling microscopy (STM), since the Si substrates used for high quality STM imaging and patterning need to be lightly doped (typically 10^{15} cm^{-3}). Electrical measurements of the final devices are therefore performed at low temperatures (e.g., <40 K for a substrate doping of 10^{15} cm^{-3}, see Ref. 14) to eliminate the effect of substrate conduction. However, at low temperatures, quantum interactions between the conduction electrons become important.

Conventional electron-electron interaction (EEI) theory for disordered 2D systems predicts[15] a correction to the Hall coefficient R_H, which can affect the carrier density determined from measurements. Prior to this study, the impact of this EEI correction on the carrier density determined from low-temperature Hall-effect measurements for δ-doped systems, and, in particular, the Si:P δ-doped system, was not clear. Since the Hall density is most commonly used to determine the degree of dopant activation in Si:P δ-doped devices,[16–19] a thorough understanding of how EEI impacts the Hall density and hence an analysis of dopant activation is important.

In this Brief Report, we present a systematic study of low-temperature magnetotransport in Si:P δ-doped layers with degenerate doping densities in the range $(\sim 0.2-2)\times 10^{14}$ cm^{-2}, from just above the transition to strong localization to the highest carrier densities achievable.[8] At low temperatures (0.3–4.2 K), we observe a temperature dependent correction in R_H consistent with conventional EEI theory for disordered 2D conductors.[15] Although such a correction has been observed in higher quality modulation doped GaAs-based 2D systems[20,21] and in Si inversion

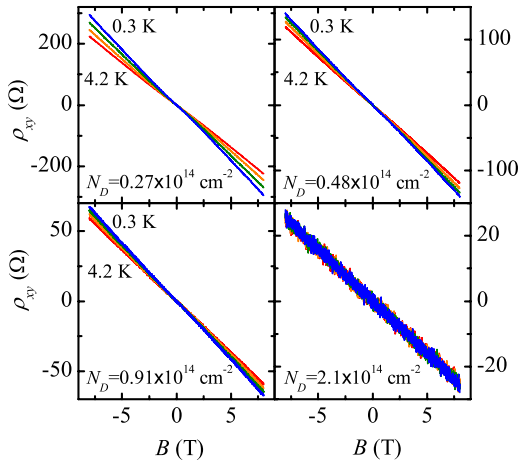

FIG. 1. (Color online) Plots of the Hall resistivity ρ_{xy} as a function of perpendicular magnetic field B for Si:P δ-doped samples at temperatures of 0.3, 0.7, 1.6, and 4.2 K (only four temperatures are shown here for clarity).

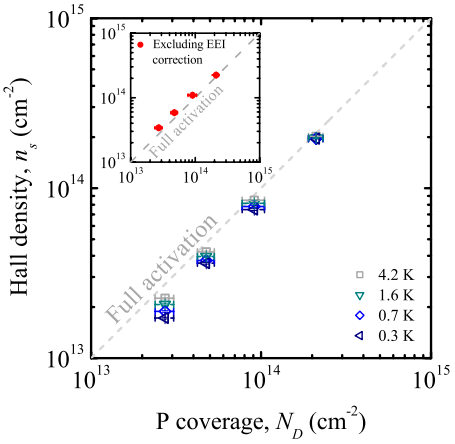

FIG. 2. (Color online) Comparison of the measured Hall densities n_s at different measurement temperatures. For clarity, only data at four temperatures are presented. Inset: Corresponding classical Hall densities (solid circles) obtained after eliminating the EEI correction from the respective Hall coefficients (note that both axes are defined in the same way as for the main graph). The dashed lines represent full electrical activation.

layers,[22] this Brief Report reports on the significance of electron-electron interactions for the more highly disordered Si:P δ-doped system. We find that the quantum correction to R_H is larger at lower doping densities and hence can potentially lead to the erroneous conclusion that the dopants are not electrically active. By modeling the correction to R_H with EEI theory, we demonstrate that it is possible to recover the classical Hall coefficient and hence the actual carrier density from our measurements. We discuss the significance of this finding in the context of analyzing dopant activation and mobility for Si:P δ-doped devices.

Four δ-doped samples were fabricated on n-type (P-doped, 10^{15} cm^{-3}) Si(100) substrates using phosphine (PH_3) gas as the dopant source and low-temperature (250 °C) Si encapsulation by molecular beam epitaxy in an ultrahigh vacuum environment. Surface doping with PH_3 was performed at room temperature and a pressure of 10^{-9} mbar, and different doping densities were achieved by varying the doping time. A detailed calibration of the doping density N_D was carried out at different PH_3 fluences using a combination of Auger electron spectroscopy and by direct counting of PH_x (x=0,1,2) features on the Si(100) surface using a STM.[8] A critical step in the fabrication of these samples is an anneal to 500 °C after PH_3 dosing in order to incorporate the P atom from the adsorbed PH_x fragment into a substitutional site in the Si(100) surface.[23] The P doping densities of the four samples determined from the combined STM and Auger analysis were 0.27×10^{14}, 0.48×10^{14}, 0.91×10^{14}, and 2.1×10^{14} cm^{-2}, with the highest doping achieved using a saturation dose[17] of PH_3. After encapsulation by epitaxial silicon, the δ-doped samples were fabricated into Hall bars for magnetotransport measurements using standard ac lock-in techniques in a dilution refrigerator equipped with a magnet for fields up to 8 T. All four samples exhibit near Ohmic conductivities from 4.2 down to 0.3 K.

Figure 1 presents the Hall resistivity ρ_{xy} data for the four samples at temperatures of 0.3, 0.7, 1.6, and 4.2 K. Here, we observe that for all samples, the Hall slope increases as the temperature is reduced. However, the magnitude of this increase becomes progressively smaller at higher carrier densities. Since the electron density is often[16–19] determined from the measured Hall slope (or Hall coefficient R_H), we present the impact of this change in R_H on the Hall density n_s and hence carrier activation in Fig. 2.

In Fig. 2, the Hall densities n_s measured at four different temperatures from 0.3 to 4.2 K are plotted as a function of the doping density N_D. Importantly, we can see that for the lowest doped sample, there is a large deviation (~50%) of n_s from the expected value assuming full electrical activation (dotted line in Fig. 2) at the lowest temperature. In contrast, for the highest doped sample, the Hall density is in reasonable agreement with the dopant density within the measurement error[8] of ~10%. At first glance, we might attribute the lower than expected n_s observed to the lack of dopant activation. Dopant complexes have commonly been implicated for dopant deactivation giving rise to a saturation of the free carrier density in highly doped semiconductors.[24–26] We note, however, that our highest doped (2.1×10^{14} cm^{-2}) sample still exhibits complete electrical activation. It is therefore unlikely that the apparent deactivation for our lower doped samples is caused by dopant complexes. Gossmann and Unterwald have previously attributed an apparent reduced activation in Si:Sb and Si:B δ-doped samples to the effects of carrier confinement within the potential well of the doping spike.[5] However, their measurements were performed at room temperature and 77 K where EEI effects are known to be small. We will show below that the apparent lower activation, which is more significant in our lower doped samples, is, in fact, caused by the EEI correction to R_H.

In order to analyze the observed temperature dependence of n_s, we first recall that the classical Hall density n_s^o is related to the classical Hall slope and/or coefficient R_H^o by

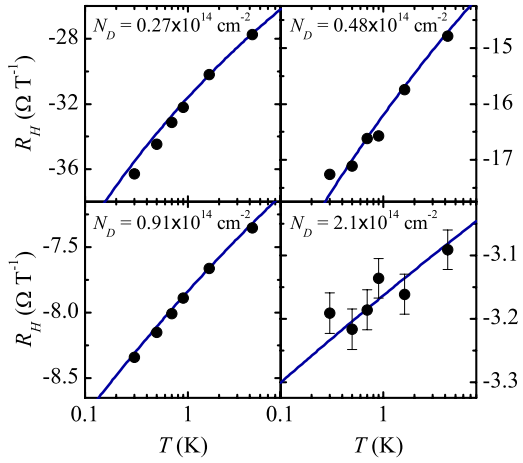

FIG. 3. (Color online) Semilogarithmic plots of the measured Hall coefficient R_H vs temperature T for Si:P δ-doped samples with different doping densities. Lines are fits to the data using electron-electron interaction theory [Eq. (3)] described in the text.

$$R_H^o = -\frac{1}{n_s^o e}. \tag{1}$$

In Fig. 3, we plot the experimental R_H as a function of temperature T on a semilogarithmic plot for each of the four samples. In contrast to R_H^o, which is independent of T [see Eq. (1)], we observe that R_H increases in magnitude as T decreases and the percentage change in R_H is significantly larger at low doping densities. In addition, the almost linear trends in Fig. 3 suggest that R_H varies as $\sim \ln T$ for all samples.

For disordered 2D systems, EEI theory predicts a quantum correction in the longitudinal conductivity σ_{xx}, which, to first order perturbation, is given by[15]

$$\delta\sigma_{ee} = K_{ee} G_o \ln \frac{kT\tau}{\hbar}, \tag{2}$$

where K_{ee} is a prefactor dependent on the screened Coulomb interaction, $G_o = e^2/\pi h$, and τ is the transport relaxation time. Note that Eq. (2) is only valid for diffusive transport ($kT\tau \ll \hbar$). As EEI does not produce any correction in the 2D Hall conductivity σ_{xy}, the $\ln T$ dependence in Eq. (2) propagates via tensor inversion into both the longitudinal resistance ρ_{xx} and Hall resistance $\rho_{xy}(=-R_H B)$. In particular, the Hall coefficient including the EEI correction δR_H may be expressed as

$$R_H = R_H^o + \delta R_H = \frac{\rho_{xy}}{B} = -\frac{\sigma_{xy}/B}{(\sigma_o + \delta\sigma_{ee})^2 + \sigma_{xy}^2}, \tag{3}$$

where $\sigma_{xx} = \sigma_o + \delta\sigma_{ee}$, σ_o is the 2D Drude conductivity, and σ_{xy} here is simply the classical Hall conductivity since there is no EEI correction in σ_{xy}. For low mobility 2D systems (such as our δ-doped samples), $\sigma_{xy} \ll \sigma_{xx}$ in the low B field regime, and Eq. (3) reduces to

$$R_H = R_H^o \left(1 + \frac{\delta\sigma_{ee}}{\sigma_o}\right)^{-2}. \tag{4}$$

A further approximation for small $\delta\sigma_{ee}/\sigma_o$ then leads to the usual expression[15]

$$\frac{\delta R_H}{R_H^o} = -\frac{2\delta\sigma_{ee}}{\sigma_o}, \tag{5}$$

and in combination with Eq. (2), we obtain

$$R_H = R_H^o \left(1 - \frac{2K_{ee}G_o}{\sigma_o} \ln \frac{kT\tau}{\hbar}\right), \tag{6}$$

which implies that R_H varies as $\sim \ln T$ and is dependent on the doping density in some nontrivial way since the parameters R_H^o, σ_o, and K_{ee} are all dependent on the doping level. Note that we have neglected weak localization (WL) corrections in the above discussion, since in the commonly assumed first order perturbation, WL does not produce a correction in R_H.

Equation (6) appears to be a straightforward way to model the apparent $\sim \ln T$ dependence of R_H observed for our samples. However, the change in R_H with T is $\sim 15\%$ or more for our lower doped samples, and the use of Eq. (6) can introduce significant errors since higher order terms have been neglected in deriving this equation. For large corrections, (i) higher order perturbation terms may need to be included in Eq. (2) if their corresponding prefactors are nonvanishing[27] and (ii) higher order terms in the series expansion of $(1+\delta\sigma_{ee}/\sigma_o)^{-2}$ need to be included in Eq. (5) and hence in Eq. (6).

While the first order perturbation term given by Eq. (2) is well known for disordered 2D systems, the corresponding higher order corrections are less obvious and may arise directly from EEI or the interplay between EEI and WL[27,28] and are beyond the scope of this Brief Report. We therefore assume Eq. (2) for our analysis but caution that this could introduce errors when $\delta\sigma_{ee}/\sigma_o$ is large.

In contrast, the series expansion in Eq. (5) can be avoided by considering Eq. (3) directly. This has recently been demonstrated by Minkov *et al.* who were able to analyze data with $\delta R_H/R_H \sim 30\%$.[21] In this method, if the correct $\delta\sigma_{ee}$ is subtracted from σ_{xx} and tensor inversion is performed to obtain the 2D resistivity tensor, one should find that the EEI-related corrections in $\rho_{xx}(B,T)$ and $\rho_{xy}(B,T)$ disappear. Specifically, (i) all the corrected $\rho_{xy}(B,T)$ traces should fall on the same line with the same Hall coefficient, and (ii) all the corrected $\rho_{xx}(B,T)$ traces should overlap in the low field regime ($B \ll 1/\mu$, where μ is the mobility) where WL is suppressed. The fitting procedure is therefore based on optimizing the elimination of the EEI correction from the resistivity tensor by systematically adjusting K_{ee} and self-consistently determining τ from the corrected resistivity tensor in each iteration.[21,29]

Using the above fitting procedure, we found K_{ee} values of 0.75, 0.90, 0.99, and 0.87 with corresponding τ values of 9.6, 8.3, 6.4 and 6.4 fs for the samples with doping of 0.27×10^{14}, 0.48×10^{14}, 0.91×10^{14}, and 2.1×10^{14} cm^{-2}, respectively.[30] In all calculations, we assumed[8] a single-

subband model with an electron effective mass of $0.315m_e$, where m_e is the electron rest mass. The K_{ee} values obtained here are in good agreement with respective values of 0.72, 0.75, 0.79, and 0.83 from theory.[31] The close agreement of the K_{ee} values extracted from our data with those predicted by 2D theory suggests that our simplified analysis including only the first order correction given by Eq. (2) is reasonable (slight differences may be due to the neglect of higher order perturbation terms in $\delta\sigma_{ee}$ and our single-subband and effective mass approximations). In Fig. 3, we plot the $R_H(T)$ curves derived from this fitting procedure. The good fit of the $R_H(T)$ curves to our data suggests that the T dependent corrections in R_H observed here can be accounted for by conventional EEI theory as long as the series expansion inherent in Eqs. (5) and (6) is avoided.

For all samples, we determined the classical Hall coefficient R_H^o by adjusting K_{ee} so that all the $\rho_{xy}(B,T)$ traces collapsed onto a common Hall slope with a single value of K_{ee}. In the inset of Fig. 2, we plot the classical carrier density n_s^o (red solid circles) obtained from the corresponding R_H^o for each sample. Using this analysis, we find classical Hall densities which are in good agreement with the respective dopant densities, suggesting full donor activation over the whole range of carrier densities. These results highlight that for the degenerately δ-doped layers studied here, we achieve full activation at all dopant densities up to the highest density obtained by saturation dosing with PH_3. In addition, the results also demonstrate the importance of using EEI theory to extract reliable carrier densities from Hall-effect measurements carried out at low temperatures.

In conclusion, we have shown that at temperatures of 0.3–4.2 K, Si:P δ-doped layers with degenerate doping densities in the range $(\sim 0.2-2)\times 10^{14}$ cm^{-2} exhibit temperature dependent corrections in the Hall coefficient R_H which can be consistently accounted for by EEI theory.[15] We demonstrate that this correction can result in a significant increase in the magnitude of the Hall coefficient (hence in an apparent decrease in the Hall density) at temperatures below 4.2 K, especially for δ layers with lower doping densities. The implication of this finding is that for such degenerately δ-doped layers, the Hall density measured at low temperatures *always* appears lower than the actual carrier density. The EEI correction to the Hall density accounts for the difference, such that for the range of densities studied, from just above the transition to strong localization to a saturation dose of $\sim 2\times 10^{14}$ cm^{-2}, the P dopants are completely active. These results demonstrate that if electron-electron interactions are unaccounted for, significant errors can occur in the calculation of electrical activation and other transport parameters such as the carrier mobility, especially at lower doping densities.

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[30] We found that if Eq. (6) was used to model our data, the K_{ee} values for our two lowest doped samples (0.27×10^{14} and 0.48×10^{14} cm^{-2}) are overestimated by ~30% and ~13% respectively, while those for the two higher doped samples (0.91×10^{14} and 2.1×10^{14} cm^{-2}) are in agreement within 10%, in comparison to using Eq. (3). Within an error of 10%, the $\sim \ln T$ dependence of R_H [Eq. (6)] is therefore valid for the two higher doped samples.
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