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Limitations to the room temperature mobility of two- and three-dimensional electron liquids in SrTiO₃

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We analyze and compare the temperature dependence of the electron mobility of two- and three-dimensional electron liquids in SrTiO₃. The contributions of electron-electron scattering must be taken into account to accurately describe the mobility in both cases. For uniformly doped, three-dimensional electron liquids, the room temperature mobility crosses over from longitudinal optical (LO) phonon-scattering-limited to electron-electron-scattering-limited as a function of carrier density. In high-density, two-dimensional electron liquids, LO phonon scattering is completely screened and the mobility is dominated by electron-electron scattering up to room temperature. The possible origins of the observed behavior and the consequences for approaches to improve the mobility are discussed. © 2015 AIP Publishing LLC.

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Two-dimensional electron liquids (2DELs) in SrTiO₃ have generated significant interest for the study of low-dimensional correlation physics^{1–6} and for novel device applications.^{7–10} At polar/non-polar interfaces, charge densities can be as high as $3 \times 10^{14} \text{ cm}^{-2}$.^{11,12} Such sheet carrier concentrations are at least an order of magnitude larger than those that can be achieved in conventional semiconductor two-dimensional electron gases. The high dielectric constant of SrTiO₃ facilitates the modulation of such large charge densities by an external electric field,^{9,10,13} making SrTiO₃ 2DELs of interest for applications in power electronic or tunable plasmonic devices. Device performance will, however, be limited by the low room temperature mobility (μ) of electrons in SrTiO₃, which is less than $10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. For example, the Baliga power device figure of merit¹⁴ is $\epsilon \mu E_g^3$, where ϵ is the dielectric constant and E_g is the band gap. For SrTiO₃, it is already fairly high, due to its wide band gap and large dielectric constant, and relatively small gains in μ could make it comparable to other materials currently being investigated for power electronic devices.

To improve transport, it is important to understand the reasons for the low mobility. For doped bulk SrTiO₃, it has long been known that the mobility at temperatures $T > 200 \text{ K}$ is limited by scattering from longitudinal optical (LO) phonons.^{15–17} At intermediate temperatures ($T \sim 20 \text{ K} - 130 \text{ K}$), the resistivity has a T^2 dependence, indicative of electron-electron scattering.^{18,19} The resistance of high-density 2DELs at $R\text{TiO}_3/\text{SrTiO}_3$ interfaces ($R = \text{La, Nd, Gd, or Sm}$), which exhibit charge densities of $\sim 3 \times 10^{14} \text{ cm}^{-2}$, follows T^2 dependence over a much wider temperature range.^{23,20} This suggests that different mechanisms determine the room temperature mobility in bulk and 2DELs in SrTiO₃ and that electron-electron interactions are significantly stronger in extreme-density 2DELs. In this letter, we analyze and compare the contributions to the room temperature mobility for the two cases. We show that LO phonon scattering is absent in the 2DELs even at room temperature.

For bulk SrTiO₃, a crossover in the limiting scattering mechanism is observed as a function of carrier density.

Epitaxial SrTiO₃ films were grown doped with different amounts of La by molecular beam epitaxy (MBE), with the three-dimensional carrier densities (N) ranging between $\sim 8 \times 10^{17} \text{ cm}^{-3}$ and $\sim 2 \times 10^{20} \text{ cm}^{-3}$. Details of the growth and results from electrical measurements are described in Ref. 21. 2DELs were formed at MBE-grown GdTiO₃/SrTiO₃ interfaces, as described elsewhere,^{11,22} and the electrical data analyzed here were previously reported in Ref. 11. The thickness of the SrTiO₃ layer, in which the 2DEL resides, was varied between 2 and 88 nm. At least 50% of the carriers in such 2DELs reside in highly confined d_{xy} states within a few nm of the interface.^{23–26} Decreasing the SrTiO₃ layer thickness increases the 3D carrier density in the layer when the layer thickness becomes comparable or smaller than the spatial extent of the 2DEL.

Figure 1(a) shows the Hall mobility (μ) of lightly La-doped SrTiO₃ ($N \sim 8 \times 10^{17} \text{ cm}^{-3}$) as a function of temperature.²¹ In the following, we describe the temperature dependence of μ by accounting for three dominant scattering mechanisms, whose reciprocals add according to Matthiessen's rule:

$$\mu^{-1} = \mu_0^{-1} + \mu_{e-e}^{-1} + \mu_{\text{LO}}^{-1}. \quad (1)$$

The three terms in Eq. (1) are: μ_0 , the low-temperature limit of the mobility, determined by ionized impurity scattering (or interface roughness scattering in case of the 2DELs); μ_{e-e} , the electron-electron scattering limited mobility; and μ_{LO} , the LO phonon limited mobility. The temperature dependence of μ_{e-e}^{-1} is given by $\mu_{e-e}^{-1} = \alpha T^2$, where α is a measure of the strength of electron-electron scattering.²⁷ The temperature dependence of μ_{LO} can be described as follows:^{15,28}

$$\mu_{\text{LO}} = \frac{K_{\text{LO}}}{\hbar \omega_{\text{LO}}} \left(\exp\left(\frac{\hbar \omega_{\text{LO}}}{k_B T}\right) - 1 \right), \quad (2)$$

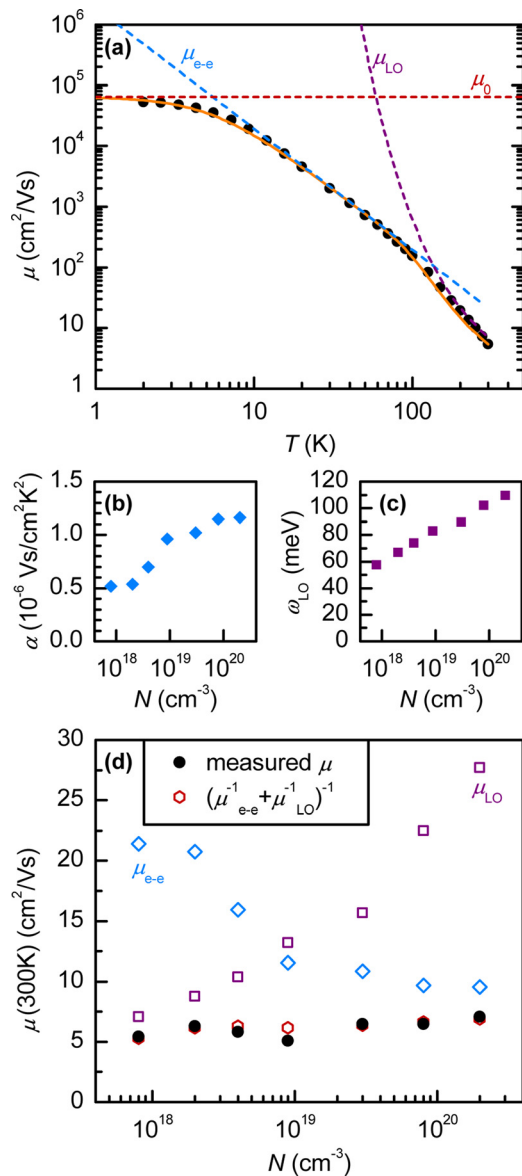


FIG. 1. (a) Temperature dependence of the Hall mobility (μ) of SrTiO₃ doped with La to a carrier density of 8×10^{17} cm⁻³ (from Ref. 21). The solid line is a fit to Eq. (1), with $\mu_{e-e}^{-1} = \alpha T^2$ and μ_{LO} as given by Eqs. (2) and (3), while the dashed lines show the temperature dependence of the terms in Eq. (1) obtained from the fit. (b) and (c) Extracted parameters α and ω_{LO} from fits to the samples with different doping concentrations (N). The individual fits are shown in the supplementary material.³⁰ (d) Comparison of the measured room temperature mobility (solid circles), μ_{e-e} (diamonds), and μ_{LO} (squares) calculated using the extracted fit parameters, and $(\mu_{e-e}^{-1} + \mu_{LO}^{-1})^{-1}$ (hexagons). The close agreement between the measured μ and $(\mu_{e-e}^{-1} + \mu_{LO}^{-1})^{-1}$ shows that the room temperature mobility is controlled by electron-electron and LO phonon scattering terms, with a crossover in the dominant contribution near $N \sim 6 \times 10^{18}$ cm⁻³.

with

$$K_{LO} = \frac{\hbar}{2\beta\hbar\omega_{LO}} \frac{e}{m_p} \left(\frac{m_e}{m_p}\right)^2 f(\beta), \quad (3)$$

where \hbar is the reduced Planck's constant, e is the electron charge, k_B is the Boltzmann constant, $\hbar\omega_{LO}$ is the energy of the LO phonon, β is the electron-phonon coupling constant, m_e is the electron effective mass (taken to be 1.8 times the free electron mass²⁹), $m_p = m_e(1 + \beta/6)$ is the polaron mass, and $f(\beta)$ is a function with a value of approximately one.²⁸ K_{LO} is approximately 0.12 eV cm²/V s, see Ref. 28.

The solid line in Fig. 1(a) shows a fit using Eqs. (1)–(3), which accurately describes the experimental data. The fit parameters were μ_0 , α , and ω_{LO} . In SrTiO₃, carriers are believed to couple strongly to two LO phonon modes¹⁸ and the value for ω_{LO} determined here is an average, effective value. Fits for the more highly doped samples are shown in the supplementary material³⁰ and yield similarly good descriptions. Figures 1(b) and 1(c) show the results for α and ω_{LO} as a function of N . As N increases, ω_{LO} and α both increase. As a result, μ_{LO} increases while μ_{e-e} decreases and the total mobility becomes increasingly limited by electron-electron scattering. This is summarized in Fig. 1(c), which shows μ_{e-e} and μ_{LO} calculated at room temperature using the extracted values for α and ω_{LO} , the total mobility calculated using these two terms, and the experimentally measured Hall mobility. At $N \sim 6 \times 10^{18}$ cm⁻³, the electron-phonon scattering limited regime crosses over to an electron-electron scattering limited regime; as a result, the mobility remains < 10 cm² V⁻¹ s⁻¹ for all N .

The increase of μ_{LO} with N is in agreement with first-principles calculations,¹⁷ where it has been shown that the electron-phonon scattering rates decrease away from the Brillouin zone center. Thus with increasing N , as the Fermi surface enlarges, the scattering rate becomes smaller, leading to an increase in μ_{LO} .

The results shown in Fig. 1 confirm earlier results that electron-electron scattering must be accounted for in describing the temperature-dependence of the mobility of SrTiO₃,¹⁸ and furthermore show that it becomes the limiting mechanism at high doping. It is well known that for simple metals with a single conduction band, electron-electron scattering leads to resistance only for Umklapp processes at linear order transport theory.^{27,31} This is due to the fact that the total crystal momentum is conserved in an electron-electron scattering event for normal (non-Umklapp) processes. In SrTiO₃, the increased electron-electron scattering rate at high doping [Fig. 1(b)] can also be attributed to Umklapp processes. With increasing N the Fermi surface expands, reaching closer to the Brillouin zone boundaries, enabling Umklapp scattering. Furthermore, when there are multiple conduction bands, as is the case for SrTiO₃,^{32,33} electron-electron scattering can proceed through both intraband and interband transitions. For an interband scattering event, the total current can change via transfer of electrons between bands with different effective masses, leading to resistance from electron-electron scattering even for normal processes, in addition to Umklapp ones.³⁴ This leads to an increased electron-electron scattering rate compared to simple metals. In addition, short-range Coulomb interactions are strong for the conduction bands derived from the localized 3d orbitals of Ti, which also leads to an enhancement of electron-electron scattering.² These interactions increase with N (as the probability of two electrons occupying the same site increases).

Figure 2 shows the Hall mobility as a function of temperature for the 2DELs in structures with different SrTiO₃ thicknesses. As shown by the dashed lines, the mobility can be completely described over the entire temperature range up to room temperature as $\mu^{-1} = \mu_0^{-1} + \mu_{e-e}^{-1}$. Thus, unlike for bulk doped samples, there is no detectable LO phonon

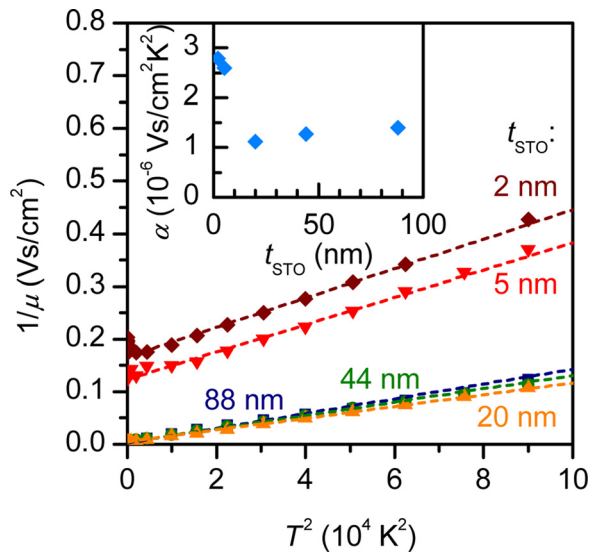


FIG. 2. Temperature dependence of the inverse of the mobility μ in 2DELS at GdTiO₃/SrTiO₃ interfaces. The samples consisted of epitaxial bilayers with SrTiO₃ different thicknesses (GdTiO₃ is the top layer) on an insulating substrate, from Ref. 11. The inset shows the extracted parameter α from fits to $\mu^{-1} = \alpha T^2$.

scattering contribution in the 2DELS. The absence of LO phonon scattering explains the slightly larger room-temperature mobility in the 2DELS. The inset in Fig. 2 shows α as a function of SrTiO₃ thickness. For the thinnest layers, the three-dimensional carrier density in the 2DEL is increased (the layer width is substantially smaller than the spatial extent of the 2DEL) and the strength of electron-electron scattering (α) is increased.

The results indicate a complete screening of the LO phonon mode in the 2DELS. In addition to the screening by the large density of carriers in the 2DEL, electronic screening also depends on the density of states (DOS). Confinement in a 2DEL increases the DOS at the Fermi level.³⁵ An indicator of a substantial increase of the DOS in GdTiO₃/SrTiO₃ 2DELS is the observed itinerant ferromagnetism,³⁶ as it is required to satisfy the Stoner criterion to cause spin polarization in the conduction bands.³⁷ Once the conduction electrons screen the ionic potentials effectively, there is no long range Coulomb interaction that splits the LO and TO mode frequencies, and therefore the polar optical mode scattering disappears, explaining the disappearance of the LO phonon scattering in the 2DEL.

Figure 3 summarizes the findings by showing the room temperature values of μ as a function of α for the 2DELS and the bulk doped SrTiO₃ samples. The dotted line indicates the electron-electron scattering limited mobility, calculated as $\mu_{e-e}^{-1} = \alpha T^2$. In bulk SrTiO₃, LO phonon scattering reduces the mobility below the μ_{e-e} limit. To increase the room temperature mobility of SrTiO₃, LO phonon scattering should be suppressed. This is achieved for the 2DELS with thicker SrTiO₃, which fall on the theoretical μ_{e-e}^{-1} line. In this limit, to improve the mobility, α should be reduced. If this proves possible, significant mobility gains (by a factor of 2 or more) could be achieved with relatively small reductions in α . For the extremely confined 2DELS (few nm SrTiO₃ layers, right-most data points), other factors, including interface

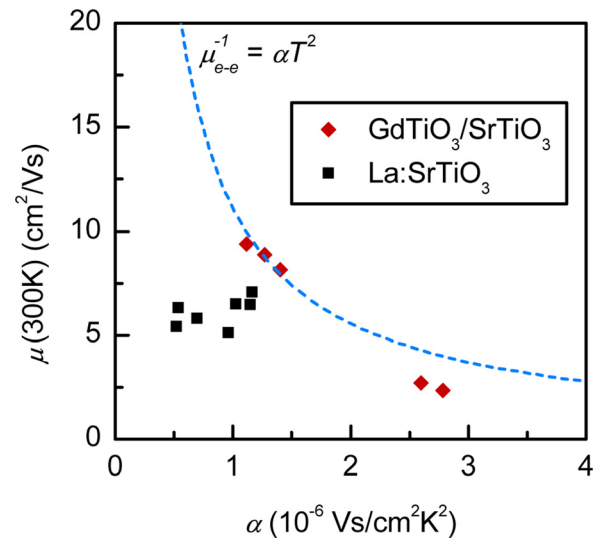


FIG. 3. Room temperature mobility as a function of the extracted electron-electron scattering parameter α for the 2DELS (diamonds) and three-dimensional electron gases (squares). The dashed line is calculated according to $\mu^{-1} = \alpha T^2$. The mobility of the three-dimensional electron gases falls below the dashed line due to the significant contribution of LO phonon scattering, which is absent in the 2DELS. The extremely confined 2DELS (two right-most data points) fall below the line due to contributions from interface roughness scattering even at room temperature.

roughness scattering, cause a drop in the mobility below the μ_{e-e} limit.

In summary, we have shown that the room temperature mobility in high-carrier-density 2DELS in SrTiO₃ is not limited by LO phonon scattering, in sharp contrast to bulk, doped SrTiO₃. To develop approaches to improve the mobility in the 2DELS, a quantitative, theoretical understanding of contributions to α in SrTiO₃ 2DELS must be developed. The results emphasize that the transport physics of 2DELS in complex oxides is significantly different from that of conventional semiconductors, where electron-phonon scattering only plays a minor role and electron-phonon scattering is the dominant mechanism limiting the room temperature mobility.

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