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Enhancing the electron mobility of $SrTiO_3$ with strain

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We demonstrate, using high-mobility $SrTiO_3$ thin films grown by molecular beam epitaxy, that stress has a pronounced influence on the electron mobility in this prototype complex oxide. Moderate strains result in more than 300% increases in the electron mobilities with values exceeding 120 000 $cm^2/V\,s$ and no apparent saturation in the mobility gains. The results point to a range of opportunities to tailor high-mobility oxide heterostructure properties and open up ways to explore oxide physics. © *2011 American Institute of Physics*. [doi:10.1063/1.3571447]

Mobility engineering using strain is widely used in semiconductor devices.[1,2] For example, compressing the channel in silicon field effect devices results in up to fourfold enhancement in the hole mobility,[1] making strain engineering the most important reason for continued performance gains in the latest generations of silicon field effect devices. Concepts that are central to conventional semiconductor devices, such as two-dimensional (2D) electron gases and field effect, are now being realized in complex oxides.[3,4] In contrast to conventional semiconductors, for which the effects of strain have been studied for decades,[5,6] mobility engineering has not yet been explored for complex oxides, such as $SrTiO_3$.

Strain has the most dramatic effects on band structure at points in reciprocal space, where electron states are orbitally degenerate. The conduction band of $SrTiO_3$, a prototype high-mobility complex oxide, is derived from Ti 3*d* states and essentially has a twofold orbital degeneracy at the conduction band minimum, resulting in "heavy electron" (HE) and "light electron" (LE) bands [Fig. 1(a)]. At 110 K, cubic $SrTiO_3$ undergoes a phase transition to a tetragonal phase, which causes splitting of the HE and LE conduction bands [Fig. 1(b)].[7,8] The manifold of states resembles in many ways the states in conventional semiconductors, such as Si, Ge, or GaAs, at the top of the valence band. In these semiconductors, a compressive, uniaxial stress along the transport direction results in valence band splitting and warping, reducing the effective mass and causing dramatic gains in the hole mobility.[1] Although the details of the conduction band structure for $SrTiO_3$ are still under debate,[7–10] the similarity of the *d*-band electron states in $SrTiO_3$ to the hole systems in conventional semiconductors motivated the present study of the effects of a compressive uniaxial strain on the electron mobility of $SrTiO_3$.

Epitaxial La-doped $SrTiO_3$ films were grown by molecular beam epitaxy as reported elsewhere.[11–13] Two samples with different effective electron densities, $n_{3D}=3.6\times10^{17}$ cm^{-3} and $n_{3D}=7.5\times10^{17}$ cm^{-3}, as determined from the Hall resistance, were used in this study. The La-doped layer thicknesses were 1280 nm and 800 nm, respectively. The sheet resistance R_S and the carrier concentrations were obtained as a function of temperature down to 1.8 K using a physical property measurement system (PPMS, Quantum Design). Measurements were made in Hall bar geometry with rectangular shaped samples (10 mm$\times$4 mm). Ohmic contacts were Al(40 nm)/Ni(20 nm)/Au(150 nm) deposited by electron beam evaporation through a shadow mask. The longitudinal and transverse resistances were measured by the low frequency (17 Hz) ac technique using a current of 10 μA. For the Hall measurements the magnetic field B was varied between ±1 T. The Hall carrier concentration n_{3D} was calculated as $n_{3D}=1/(t\times e\times R_H)$, where t is the thickness of the doped layer, R_H the measured 2D Hall coefficient and the Hall scattering factor was assumed to be unity. The Hall carrier concentration corresponded to the La dopant concentration, as reported previously.[13] The Hall mobility μ was calculated as $\mu=R_H/R_S$ and is independent of any errors in determining the film thickness.

Four-terminal magnetotransport measurements of La-doped $SrTiO_3$ layers grown on insulating $SrTiO_3$ substrates were carried out under different amounts of uniaxial, compressive stress using the three-point bending apparatus shown in Fig. 2(a). The mobilities of the samples are high

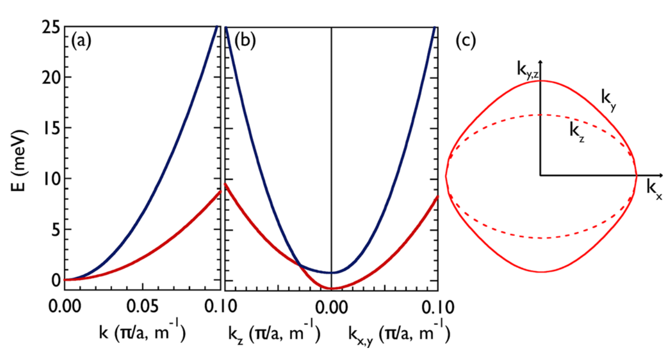

FIG. 1. (Color online) Energy bands near the conduction band minimum for the cubic and tetragonal phases of $SrTiO_3$. (a) Conduction band energy (E) vs wave vector (k) relationship of cubic $SrTiO_3$ showing degenerate (at $k=0$), HE and a LE bands. (b) The conduction bands split for tetragonal $SrTiO_3$. Along the direction of the longer tetragonal c-axis the LE band is lower in energy. The spin orbit split-off band is not shown. (c) Fermi surface of the lower band of the band structure shown in (b). The band parameters used here are obtained from an analysis of magnetoresistance oscillations by Uwe *et al.* (Ref. 8).

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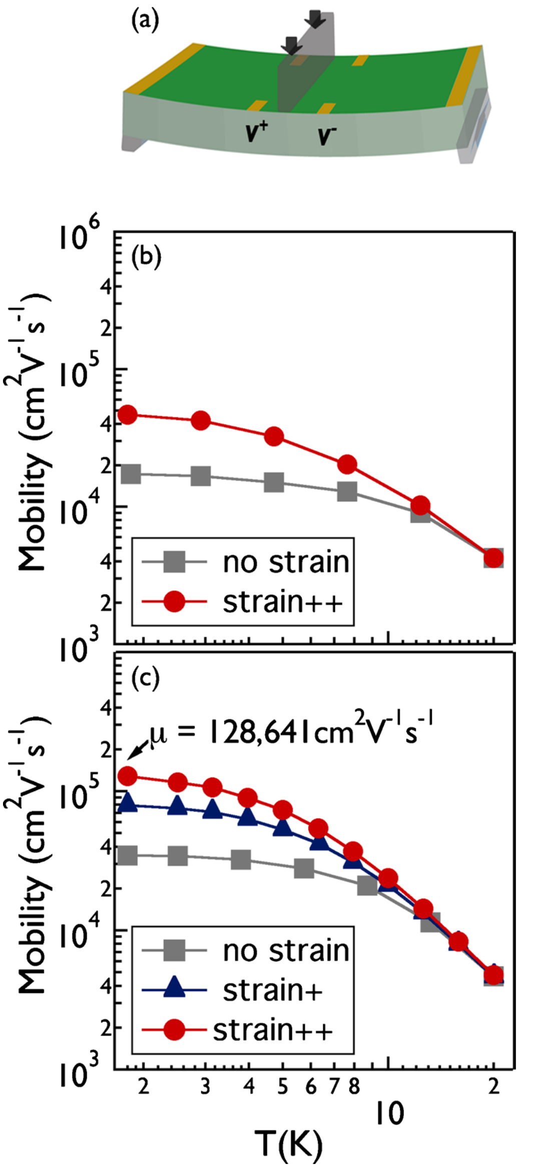

FIG. 2. (Color online) Stress-induced electron mobility gains in epitaxial $SrTiO_3$ thin films. (a) Schematic of the three-point bending apparatus. (b)–(c) Hall electron mobility (μ) in $SrTiO_3$ layers with (b) a carrier concentration of 3.6×10^{17} cm^{-3}, and (c) a carrier concentration of 7.5×10^{17} cm^{-3} as a function of temperature under different uniaxial stress.

enough to expose Shubnikov–de Haas oscillations at the lowest temperatures.[13] The direction of the compressive stress and the electron transport were along ⟨100⟩. The maximum strain along the transport direction was approximately −0.3% at the center of the sample (see Ref. 14) and thus substantially larger than the tetragonal strain that appears below the 110 K phase transition, which is on the order of 0.05%. The three-point bending setup was mounted onto a puck in the PPMS system. The strain in the epitaxial layer was estimated using estimates of the displacements and the curvature-strain relationship for the three-point bending test.[14]

Figures 2(b) and 2(c) show the electron mobility of the two different $SrTiO_3$ layers as a function of temperature under different applied stress. The lower doped sample has a lower mobility, consistent with findings in the literature for very low-doped $SrTiO_3$.[15] The mobilities increase dramatically under applied compressive stress. The mobility of the higher density sample rises by a factor of ~3.3 to 128 000 $cm^2/V\ s$ while the mobility of the lower density sample rises by a factor of ~2.5 to 46 000 $cm^2/V\ s$.

The numerical values of the Si band parameters that describe the heavy and light hole bands, and their splitting under uniaxial stress, are likely different from those that apply to the conduction band of $SrTiO_3$. However, the strong increase in mobility can be qualitatively explained following the work by Hensel and Feher on the effect of uniaxial stress on the valence band of Si.[6] The substantial increase in mobility at low carrier density is then caused by (1) removing many domains with different tetragonal distortions, (2) exclusively populating the lowest of the conduction band states in the presence of the strain, and (3) a compressive strain that leads to a light effective mass along the strain and transport directions. We next discuss these three points.

In an unstrained sample, domain formation is expected as a result of the phase transition and the transport will be an appropriate average of the transport in each kind of the domains and influenced by scattering at the domain boundaries. In the experiments reported here the induced strain along the transport direction is five to six times larger than the tetragonal strain, so that transport in a single domain, along the transport direction, is a reasonable assumption. Previous estimates of the conduction band splitting[7,8] due to the tetragonal distortion suggest that the Fermi energy for the two samples studied may well be below that needed to *solely* occupy the lower band when the films are under compressive stress, transport occurs in a single band. The highly enhanced mobility implies that under compressive stress the lower, solely occupied state has a light mass along the strain (compressive) and transport direction.

The states at the conduction band minimum in the low temperature tetragonal phase determined from single domain Shubnikov–de Haas oscillations[8] are shown in Fig. 1(b). The dispersion is similar to the calculated band structure of Mattheiss,[7] except for a substantially smaller splitting (approximately by a factor of 5). Both, however, indicate a light mass along the tetragonal *c*-axis, which is marked by a small *tensile* strain. The results here indicate that, similar to Si,[6] a *compressive* stress leads to a light mass along the stress direction. Specifically, the deformation potential is such that a large compressive strain leads to the band structure shown in Fig. 1(b) (*z*-direction), a solely occupied band for low electron densities, such as those explored here, and a Fermi surface as shown in Fig. 1(c) with light effective mass along the *z*-direction and heavy mass perpendicular to it. While at present we cannot resolve the apparent discrepancy, we note that the electron density for the samples used in the Shubnikov–de Haas experiments of Uwe *et al.*[8] occupied both bands, the Fermi energy was well above the splitting induced by the tetragonal distortion; thus further studies are needed to understand clarify the origin of the observed splitting. Furthermore, band structure calculations have shown that the displacements of the oxygen atoms in the tetragonal phase are central to the band splitting.[7] Thus the "deformation potential" assigned in the phenomenological model by Uwe,[8] which is based on the splitting of an unstrained sample, is likely not *directly* related to a true deformation potential under an externally applied stress.

A truly quantitative understanding of the strain-enhanced mobility in $SrTiO_3$ will require knowledge of deformation potentials, which are presently unknown, and sorting out the details of the electronic structure, such as the precise distortion of the energy surfaces. The complexity of the conduction band structure of $SrTiO_3$ makes such studies challenging but they are also needed to determine the effects of electric field and quantum confinement on the transport properties of $SrTiO_3$. In particular, splitting of conduction bands due to strain closely mirrors the effects of internal, vertical electrical fields, produced by quantum confinement.

In summary, enhancements of electron mobilities under uniaxial stress by more than 300% show that large gains in mobility are possible by conduction band engineering in $SrTiO_3$. Because no saturation was observed in the mobility enhancements in the experiments reported here, even larger gains in the mobility should be feasible with larger stresses that are easily achieved in heterostructures. In analogy with conventional semiconductors, appropriate biaxial stress, which can be obtained by growth on suitable lattice-mismatch substrates, are likely to produce increases in mobility for quantum confined two-dimensional electron gases.[16] We note that the fractional quantum Hall effect was discovered in a GaAs sample having a mobility of 90 000 $cm^2/V\,s$.[17] The very large mobilities, exceeding 100 000 $cm^2/V\,s$, demonstrated here, will expose lateral quantum transport such as quantum Hall effect and edge state transport in a *d*-band system.

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