

Lightly doped SrTiO₃: A challenge to conventional solid state theory

1. Heavy non-degenerate electrons in doped strontium titanate

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2. Scalable T² resistivity in a small single-component Fermi surface

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Recommended with a Commentary by Peter Wölfle, Karlsruhe Institute of Technology, Germany

Strontium titanate (STO) is a widegap semiconductor in the paraelectric phase, close to a ferroelectric instability. Its dielectric constant increases with decreasing temperature from $\epsilon_0 \approx 300$ at room temperature up to 20000 at temperatures below $T \approx 10\text{K}$ (for a review see [1]). As a consequence, screening by ionic charges is very effective at low T . When lightly n-doped (by substitution, e.g. SrTi_{1-x}Nb_xO₃, or by removing oxygen SrTiO_{3- δ}) a well defined metallic state of STO emerges over a wide range of carrier densities, down to $n \gtrsim 10^{16}\text{cm}^{-3}$. This is not surprising as the strong screening leads to a very large Bohr radius, such that a metal-insulator transition (of the carrier system) is expected only at densities as low as $n_c \approx 10^{11}\text{cm}^{-3}$. It appears that the rigid band picture using virtual crystal approximation works well [1]. Lightly doped STO at low temperatures at first sight is well accounted for by a weakly interacting Fermi liquid model, applied to a simple electronic structure of three nearly degenerate almost isotropic bands giving rise to small close to spherical Fermi surfaces centered at the Γ point. Over the last 50 years and especially recently, however, a number of unusual properties have been discovered that remain unexplained or might even give reason to expect that something entirely new is happening here.

The first remarkable deviation from conventional wisdom [Recommended Paper 1] concerns the electronic transport properties at higher temperatures, way above the Fermi temperature, up to 900K. Analyzing the electric resistivity in the usual way it is found that the mean free path l drops so fast with increasing temperature that it seems to violate the Mott-Ioffe-Regel criterion posing that $l > \lambda_F, \lambda_T$, the Fermi wave length, or the thermal de Broglie wave length (within a scattering picture the size of the smallest wave packet should be less than the mean free path). Equivalently, the transport scattering rate (at high temperature) appears to rise above the Planck limit $\hbar/\tau > k_B T$. A way out of this conundrum would be given by a carrier effective mass $m^*(T)$ increasing with temperature. Indeed, the authors of

Recommended Paper 1 found evidence for an increase of $m^*(T)$ by more than a factor of two for temperatures rising from 100K to 300K followed by a saturation, by measuring and analyzing the thermoelectric Seebeck coefficient. They show that the observed temperature dependence of the effective mass removes the conflict with the Mott-Ioffe-Regel criterion and the Planck limit up to 400K, but at the highest temperatures the conflict still exists. A possible explanation of this behavior may be found in two recent works [2], [3] exploring the consequences of a strong electron-phonon interaction at these high temperatures. These authors, employing state of the art numerical techniques, are able to show that as the temperature rises beyond the Fermi temperature Landau quasiparticles evolve into polarons the mass of which is indeed increasing with temperature. Single particle excitations appear not to exist anymore beyond a limiting temperature depending on the position in the Brillouin zone, and the system is in what is called an incoherent state. For a class of incoherent states it has been shown that the Planck limit is respected [4]. In the case of STO the incoherent state found in [2], [3] appears to violate the Planck limit, which is presumably related to the fact that "external interactions" (phonons), which are not included in the derivation of "universal bounds" [4] play the main role.

A further puzzling observation is presented in Recommended Paper 2: the electrical resistivity shows a law $\rho(T) = \rho(0) + AT^2$ at low temperatures below the Fermi temperature. This is usually attributed to electron-electron scattering, with a phase space limited by T^2 . However, e-e-scattering is momentum conserving and as such does not relax the charge current. In conventional metals umklapp processes are thought to provide the necessary transfer of momentum from the electron system to the lattice. The small Fermi surfaces found in STO do not allow umklapp scattering. Electron-phonon scattering is not an option either as it freezes out much faster than e-e-scattering and leads to a T^5 law (acoustic phonons) or exponential law $e^{-\omega_{LO}/T}$ (optical phonons). One possibility left is impurity scattering combined with e-e-scattering, although experiment seems to exclude a strong dependence on impurity concentration. At temperatures beyond the Fermi temperature, but still less than the optical phonon scale, the resistivity is found to rise faster, more like T^3 [Recommended Paper 2], posing a further puzzle. Somewhat similar behavior is found in other systems close to a ferroelectric state, such as KTaO_3 , PbSe , PbTe , suggesting that the strong screening and the soft phonon mode might play a role here [Recommended Paper 1].

The probably most spectacular property of STO is that it enters a superconducting phase at low temperatures not exceeding $T_c \approx 0.4\text{K}$ [1]. The transition temperature $T_c(n)$ as a function of carrier density n forms a "dome" reminiscent of the cuprates. Although known since the 1960 [5], a complete understanding of the superconducting state is still missing. This may appear surprising because the mechanism is most likely given by phonons. There are, however, several unusual aspects here. The first is the smallness of the Fermi energy compared to the optical phonon energy. A separation of the interaction into a phonon exchange term and a static screened Coulomb repulsion term is no longer possible. Rather, the relevant interaction is the fully dynamically screened Coulomb interaction [6]. The conflicting results for T_c obtained by several authors within this model depend on various additional approximations employed, and a consensus has not been reached yet. The observed superconductivity at the lowest densities of $n \approx 5 \times 10^{17} - 5 \times 10^{18} \text{cm}^{-3}$ for oxygen deficient $\text{SrTiO}_{3-\delta}$ is not found for Nb-doped STO, posing a further puzzle [1]. Another challenge is given by the observation of an enormous sensitivity of T_c to isotope substitution

(replacing ^{16}O by ^{18}O) or to negative (positive) pressure, causing an increase (decrease) of up to 50%, while moving the system closer to (or farther away from) the ferroelectric phase [7], [8], [9]. A likely source of this behavior is the coupling of electrons to the soft TO phonon mode, of frequency $\omega_{TO}(q)$ vanishing at the FE transition in the limit $q \rightarrow 0$ [10]. Preliminary estimates of the usual deformation potential coupling of electrons to transverse optical phonons found it to be too small to be relevant, so that identifying a sufficiently strong coupling remains an open problem.

In summary, lightly doped strontium titanate displays a number of unexpected properties calling for a reexamination of some of the well-established concepts and methods of solid state theory. The lessons that may be learned from a deeper understanding of this unusual system will surely be valuable in future studies of novel materials.

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