Hole Mobility and Antiferromagnetic Correlations in Underdoped $La_{2-x}Sr_xCuO_4$ High-T_c Cuprate Explained

In order to better understand the origin of high-T_c superconductivity, researchers at the Central Research Institute of Electric Power Industry in Tokyo, Japan, have systematically studied the doping dependence of the mobility of holes in underdoped high-T_c cuprates. Specifically, the research group has examined the moderately to heavily underdoped region of the $La_{2-x}Sr_xCuO_4$ (LSCO) cuprate system. Unlike other superconductors, the underdoped region of high-T_c cuprates has many unusual properties such as log $(1/T)$ insulating behavior, charged-stripe instability, and the presence of a pseudogap. The experiments indicate that the x-dependence of the hole mobility, μ, at 300 K is strikingly similar to that of the inverse antiferromagnetic (AF) correlation length, ξ_{AF}^{-1}, which is known from neutron experiments. The researchers discuss both an incoherent-metal picture and a charged-stripe scenario as possible theories to account for the observation.

As reported in the July 2 issue of *Physical Review Letters*, the researchers prepared a series of LSCO samples using the traveling-solvent floating-zone technique. The samples were carefully annealed to remove the excess oxygen and ensure that the hole doping is identical to x. The crystallographic axes were determined, and the samples were shaped into platelets with the *ab* plane parallel to the wide face. Metallic charge transport in high-quality single crystals of LSCO was examined from lightly to optimally doped samples (x = 0.01–0.17), employing both in-plane resistivity and Hall coefficient measurements. At 300 K, the researchers found that the inverse mobility, μ^{-1}, exhibits a metallic temperature dependence, throughout the underdoped region, down to x = 0.01 and is weakly dependent upon x, changing by only a factor of three from x = 0.01 to x = 0.17. The researchers said that this result is interesting since a superconductor-insulator transition occurs at approximately x = 0.05. Moreover, the researchers discovered that the x-dependence of μ^{-1} is analogous to that of ξ_{AF}^{-1} in the whole underdoped region. According to the researchers, this is a notable similarity since there exists in this region a significant change in the ground state. This implies that the mechanism which governs the charge transport is the same from x = 0.01 to x = 0.17 and is related fundamentally to the background AF correlations. Although the idea of an incoherent metal accounts for some of the observed results, the connection between the x-dependence of μ^{-1} and ξ_{AF}^{-1} is better explained within the charge stripe scenario.

"Actually, the lightly doped LSCO crystals show a number of surprising features in both the transport and the magnetic properties," said Yoichi Ando, leader of the group, "and the result we report here suggests that the physics responsible for the lightly doped region is also responsible for the high-T_c superconductivity at x = 0.17."

JENNIFER L. BURRIS

Ab Initio Calculations Explain Differences in (111) Surface Reconstructions of Diamond, Silicon, and Germanium

Friedhelm Bechstedt and co-workers at the Institut für Festkörpertheorie und Theoretische Optik at Friedrich-Schiller-Universität have performed an *ab initio* investigation of the (111) surface reconstructions for carbon, silicon, and germanium in order to explain their differences. As reported in the July issue of *Physical Review Letters*, using a plane-wave, pseudopotential implementation of density-functional theory within the local-density approximation, the researchers provide insight into the nature of the reconstructed surfaces by comparison of relative energetics, optimized surface geometries, and analysis of the electronic structure for each system.

The researchers studied the structures of the 2×1, $c(2 \times 8)$, and 7×7 reconstructions of the (111) surface for each of diamond, silicon, and germanium. They performed calculations for all three elemental solids on an equal theoretical footing, allowing direct identification of the differences in surface properties and providing the first-known reported comprehensive understanding of the underlying driving forces leading to the observed differences in reconstruction behavior with diamond favoring 2×1, silicon favoring 7×7, and germanium equally favoring 7×7 and $c(2 \times 8)$. Carbon, silicon, and germanium have the same valence electron configuration. Nevertheless, carbon's strong localized bonds and lack of p and d core electrons result in markedly different reconstruction properties. The strong bonds of carbon inhibit the long-range reconstructions induced by adatoms that are energetically favorable for both silicon and germanium. As expected, silicon exhibits behavior intermediate to that of carbon and germanium.

"Although certain aspects of these surface reconstructions have been understood for decades, it is satisfying to uncover aspects of the underlying mechanisms leading to the most energetically favorable surface structures in each case," said Bechstedt. "This work provides a succinct foundation for understanding differences in the important (111) surface reconstructions for elemental semiconductors, a subject of interest to both fundamental physical understanding and practical application."

EMILY JARVIS

Dendrimers Facilitate Two-Photon Absorption Applications

Two-photon absorption (TPA) is a third-order nonlinear optical process which could be used for various optical applications, including optical memory or optical power limiting, if the available nonlinear optical materials such as organic molecules could offer higher values of nonlinear absorption cross section (σ_2) than currently observed. A team of researchers from Montana State University has reported in the July 15 issue of *Optics Letters* that dendrimers based on 4,4′-bis(diphenylamino)stilbene (DPAS) repeating units have a TPA cross section of 11×10^3 GM (1 GM = 10^{-50} cm^4 s molecule^{-1} photon^{-1}), which is the highest recorded for a monodisperse organic macromolecule. The researchers said that the TPA cross section is a factor of three larger than the previous largest TPA cross section and is a factor of 1000–10,000 times those of conventional organic dyes.

DPAS is a D-π-D-type TPA active chromophore in which D symbolizes electron donating and π stands for π conjugation. Three generations of dendrimer macromolecules with 5, 13, and 29 DPAS units were fabricated. The dendrimer's three-dimensional structure affords a high-packing density of chromophores per unit volume and stable photochemical and thermal performance, as well as the possibility for chemical modification.

Femtosecond fluoresence spectroscopy was used to measure both single-photon and two-photon absorption properties of the dendrimers. From the TPA spectra in the three consecutive generations of DPAS dendrimer macromolecules, the researchers observed that at the wavelength of 714 nm, the dendrimers' intrinsic σ_2 values increased linearly with the total number of stilbene chromophores. Most significantly, for the second generation of the dendrimer possessing 29 stilbene chromophores, σ_2 reached the value of 11,000 GM. The researchers also reported that DPAS dendrimers had high quantum yields of fluorescence, which would be important for the application of TPA.

The researchers speculate that larger σ_2 values in higher generations of this den-

drimer family will be obtainable, which will facilitate practical applications for TPA molecules.

YUE HU

Anomalous Behavior Observed in the Magnetic State of Untwinned Lightly Doped $La_{2-x}Sr_xCuO_4$ Single Crystals

Researchers from the Central Research Institute of Electric Power Industry in Tokyo, Japan, have found unusual behavior in the magnetic susceptibility in detwinned $La_{2-x}Sr_xCuO_4$ (x = 0–0.03), or LSCO, single crystals. Parent insulating cuprates at high temperatures are considered to be two-dimensional (2D) Heisenberg antiferromagnets. The presence of doped holes introduces frustration into the spin system, and it has been postulated that, for the lightly doped region, the doped holes are distributed homogenously. A consequence of this homogenous picture is that once the long-range antiferromagnetic (AF) order is destroyed due to hole doping, the spin system must be isotropic. In the July 2 issue of *Physical Review Letters*, A.N. Lavrov, Y. Ando, S. Komiya, and I. Tsukada present a detailed study of the static magnetic susceptibility (χ) in LSCO crystals in the lightly doped region that demonstrates anisotropies in the "paramagnetic" state that are inconsistent with this picture of a 2D Heisenberg antiferromagnet. Their study of the low-temperature spin freezing in these untwinned crystals also reveals an anisotropic Curie constant and anisotropic "spin-glass" temperature.

Parallelepiped samples of LSCO single crystals (~40 mg) were prepared such that all faces coincided with the orthorhombic crystal planes to within 1°, and the samples were annealed in helium to remove excess oxygen. To obtain untwinned crystals, the samples were cooled slowly under a uniaxial pressure of 15–30 MPa. X-ray analysis and magnetic susceptibility measurements were performed to measure the detwinning in the bulk, and the fraction of misoriented domains was estimated to be below 5%. The researchers used a superconducting quantum interference device (SQUID) magnetometer at fields ranging from 0.2 kOe to 5 kOe applied along the orthorhombic crystal axes, *a* and *b* (*c* axis normal to the CuO_2 planes).

Magnetic susceptibility was measured as a function of temperature along the *a*, *b*, and *c* axes in undoped (x = 0) AF samples. While the χ_c data agreed with previous studies, the χ_a and χ_b data displayed unexpected results, including a temperature dependence below the Néel temperature (T_N) and a deviation of χ_a from χ_b above ~330 K in the "paramagnetic" state. These features reveal that suppression of the long-range Néel order in undoped LSCO does not make the system isotropic. For the lightly doped (x = 0.01) AF case, the researchers observed a similar deviation between χ_a and χ_b and no sign that an isotropic spin state was recovered above T_N. Furthermore, said Lavrov, this behavior is not limited to the AF samples. Lavrov said, "We are surprised that the unexpected anisotropy persists to higher doping levels (x = 0.02, 0.03) even after the long-range AF order is expected to be destroyed due to hole doping."

The researchers report that at low temperatures in the spin-glass state, the susceptibility is also anisotropic. Upon cooling below the spin-glass temperature, χ decreases steeply, but this freezing phenomenon is more complicated than was previously thought.

"While we are exploring several possibilities and plan to conduct further studies in order to arrive at a conclusive picture," said Lavrov, "it is clear that the magnetic state in lightly doped cuprates appears to be significantly different from a simple 2D Heisenberg antiferromagnet."

STEFFEN K. KALDOR

Soft Lithography Produces Well-Aligned Carbon Nanotubes

Carbon nanotubes' (CNTs) electronic, mechanical, and chemical properties make them potential candidates for various applications. For possible nanometer-scale integrated-circuit application, it is important to develop a controlled method to synthesize high-quality CNTs. Recent research using physical masks or photo-masks have limited resolution for the resulting nanotube patterns (in micrometer scale). A team of researchers from Fudan University, China, has synthesized well-aligned CNT patterns by a soft-lithographic technique.

The support material for the catalysts is key in determining the basic parameters of CNTs, including the number of walls, the diameter, and the graphitization. As reported in the July issue of *Chemistry of Materials*, the researchers combined the micromolding in capillaries (MIMIC) technique with three-dimensional (3D) cubic mesoporous silica films containing iron nanoparticles as catalysts to fabricate carbon nanotube patterns with aligned orientations. The researchers incorporated the transition-metal catalysts into the ordered mesopores. The molecularly well-defined mesoporous silicon materials have large pores that allow efficient diffusion of species involved in the reactions and lead to high yield and purity of the nanotubes.

The researchers deposited well-aligned patterned CNTs on this catalyst film by chemical vapor deposition (CVD) with high yield (400%). Scanning electron micrographs (SEMs) show that the CNTs are almost pure and also demonstrate that the distribution of the catalyst controls the growth of CNTs. Different patterns were obtained, including striplike, petal-like, and square and hexangular patterns, by using a variety of stamps.

The CNT arrays are perpendicular to the substrate. High-resolution SEM shows that the arrays are composed of thousands of CNTs compacted together. These CNTs have a length of ~10 μm and outer diameter of about 20–40 nm. Formations of CNT arrays are related to the pore structure. On the 3D cubic-ordered mesoporous silica SBA-16 with nanopores perpendicular to the substrate, perpendicular CNTs are obtained, while the 2D hexagonal structure SBA-15 with 1D channels parallel to the substrate promotes parallel growth.

Interior and wall structure information has been acquired by transmission electron microscopy of some of the typical thinner CNTs. They have a structure with multilayer graphitized carbon walls. An increase in the amount of iron catalysts leads to a large yield of CNTs, but does not modify the diameters. Finding new catalyst support materials for CNTs with smaller diameters is still the future goal.

LI ZENG

Bubbles Simulate Atomic-Scale Contact at Surfaces

Using a raft of soap bubbles to simulate the behavior of atoms, researchers at the Massachusetts Institute of Technology (MIT) have built a macroscopic system that can provide insight into the characteristics of nanoscale contact at surfaces.

In a communication published June 7 in *Nature*, Subra Suresh, the R.P. Simmons Professor and Head of the Department of Materials Science and Engineering at MIT and his graduate students, Andrew Gouldstone and Krystyn Van Vliet, described how they created the raft of bubbles a single-layer thick to represent an atomic layer of a material's surface. Using a high-resolution digital camera, the researchers monitored, in real time, the evolution of asperity-level contact and defect nucleation when they indented the surface from the side. They then compared data from the bubble simulation with data from nanoindentation of a variety of metals.

The experiments provide quantitative information about the location beneath the contact surface where defects nucleate