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Cascade Structural Analysis and Characterization of High-Temperature Superconductivity

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ABSTRACT
To explain the reason of high temperature superconductivity phenomena and characterization of compounds having this property, various layered cuprate structures are studied step by step taking in account to their relevant critical temperatures. The substitution of Cu by particularly the 3d transition metals should produce substantial changes in the superconducting properties, which will elucidate the electronic structure, the mechanism and the possible technological applications. Understanding such defects can guide our search for new superconducting compounds. Also the modes involving oxygen motion are responsible for High Temperature Superconductivity (HTSC) mechanism.

INTRODUCTION
Since superconductivity was discovered in 1911 at 4.2 K in Hg, preparing materials with higher T_C have been a goal and a dream of scientists in this field. This has stimulated the synthesis of a lot of materials like intermetallics, low-dimension structures, organic superconductors,excitonic superconductors, superconductivity under pressure, heavy fermion systems and transition metal compounds. The T_C (23.2 K) achieved for films of Nb_3Ge, in 1973, has remained as the highest limit until 1986.

An Avalanche of research activities has resulted from the discovery of high-T_C superconductivity, in 1986, in La-Ba-Cu-O (Tc = 30 K). The discovery of Y-Ba-Cu-O in 1987 with T_C in the 90 K range surpassed the so called technological and psychological temperature barrier of 77 K, the boiling point of liquid nitrogen, and made a new leap in this field. The phase was identified as an ordered, defect perovskite structure with composition $YBa_2Cu_3O_{7-\delta}$. Further, superconductivity was achived in $RA_2Cu_3O_{7-\delta}$ (R = rare earth elements except Ce, Pr and Tb and A = Ba or Sr) and in $YBa_2Cu_4O_8$ and $Y_2Ba_4Cu_7O_{15}$ systems.

In the following years, Comounds like $Bi_2Sr_2Ca_2Cu_3O_6$ & $Bi_2Sr_2Ca_2Cu_3O_{10}$ (T_C ~ 110 K), $Tl_2Ba_2Ca_2Cu_3O_{10}$ & Tl_2 $Ba_2Ca_2Cu_3O_{10}$ (T_C ~125 K), $HgBa_2Ca_2Cu_3O_{8+y}$ system (T_C ~133 K) and $HgBa_2Ca_2Cu_3O_8$ (T_C ~133 K) were discovered. **To date, the highest Tc attained at ambient pressure has been 138 K in ($Hg_{0.8}Tl_{0.2}$) Ba2Ca2Cu3O8.33.**

Critical temperature (T_c), crystal structure and lattice constants of some high-T_c superconductors are illustrated below

Formula	Notation	T_c (K)	No. of Cu-O planes in unit cell	Crystal structure
$YBa_2Cu_3O_7$	123	92	2	Orthorhombic
$Bi_2Sr_2CuO_6$	Bi-2201	20	1	Tetragonal

Critical temperature (T_c), crystal structure and lattice constants of some high-T_c superconductors are illustrated below

Formula	Notation	T_c (K)	No. of Cu-O planes in unit cell	Crystal structure
$Bi_2Sr_2CaCu_2O_8$	Bi-2212	85	2	Tetragonal
$Bi_2Sr_2Ca_2Cu_3O_6$	Bi-2223	110	3	Tetragonal
$Tl_2Ba_2CuO_6$	Tl-2201	80	1	Tetragonal
$Tl_2Ba_2CaCu_2O_8$	Tl-2212	108	2	Tetragonal
$Tl_2Ba_2Ca_2Cu_3O_{10}$	Tl-2223	125	3	Tetragonal
$TlBa_2Ca_3Cu_4O_{11}$	Tl-1234	122	4	Tetragonal
$HgBa_2CuO_4$	Hg-1201	94	1	Tetragonal
$HgBa_2CaCu_2O_6$	Hg-1212	128	2	Tetragonal
$HgBa_2Ca_2Cu_3O_8$	Hg-1223	134	3	Tetragonal

RESULT AND DISCUSSION

Superconductivity has also been observed in the other systems, such as, Nd-(Ce, Th)-Cu-O, $Ba_{1-X}K_XBiO_{3-y}$, A_3C_{60} (A=alkali metals), $HgBa_2CuO_{4+\delta}$, MgB_2, $AuBa_2Ca_3Cu_4O_{11}$, etc.

One of the recent Y-based HTSC with Tc above 100 K is Y3Ba5Cu8O18 compound, which was synthesized and Characteristic XRD experiment was performed on the samples and was analyzed by the MAUD software refinement program. The analysis results indicate a 358 phase structure with the initial nominal stoichiometry. The electrical resistivity and its behavior under different magnetic field were measured. The electrical resistivity indicates the transition temperature Tonset c ¼ 102 K with transition width DTc = 2.4 K. This is the first observation of such a high transition temperature in the Y-based compound. Application of magnetic field leads the resistivity curve to spread out below transition region, and Tc (q = 0) shifts to lower temperatures. Also, a small broadening is observed by the application of high magnetic field in the Tonset c region.

There have been reports of superconductivity at temperatures higher than 150 K. A large number of these results are clearly due to experimental artifacts. Results, which appear to be genuine, are difficult to verify, because the superconducting component is very small and unstable.

The critical point concerned with the high-T_C cuprates is that, for transition metal oxide compounds, the parent compounds are AFM insulators. The Cu-O assembly is responsible for the superconductivity and the main contribution to the density of states, comes from the Cu 3d and O 2p hybridization states. The role of Y and Ba is helping to stabilize the structure and to the charge transfer mechanism between copper sites. As one might expect from the crystal structure, the electrical properties of the cuprates are anisotropic. The degree of anisotropy is specific to a compound family and reflects how effectively the charge reservoir layers block the coherent motion of electrons between the CuO_2 planes.

Thus, the substitution of Cu by particularly the 3d transition metals should produce substantial changes in the superconducting properties, which will elucidate the electronic structure, the mechanism and the possible technological applications. Also, understanding such defects can guide our search for new superconducting compounds.

The difficulty in understanding the HTSC arises from the fact that the exact nature of the metallic phase in the normal-state is not known. Much work is focused on whether the metallic cuprates are like ordinary metals and on those unusual properties that are unique attributes of the metallic cuprates. More important is the fact that the understanding of these materials is closely tied to the quality of experimental data and on sample quality.

The resistivity ρ appears to be close to linear over the entire normal-state regime. This indicates that phonons are not the sole source of the linear T dependence. It is unlikely that the observed strong T dependence of the inverse Hall coefficient measurements is caused by electron-phonon scattering. Also the observed carrier concentration of the charge carriers is small ($\sim 10^{21}$ cm^{-3}). Invoking more than one type of carriers (such as heavy and light electrons or holes and electrons described by different bands) to explain ρ (T) and R_H (T), would require a fortuitous and unlikely combination of temperature-dependent carrier concentrations and mobilities.

Thermopower measurements suggest that the band-filling and the phonon drag mechanisms with the involvement of two-carrier species seem operative in these superconductors. It remains to be determined whether the broad Raman scattering, which is highly characteristic of the cuprates, is due to spin or charge excitations or both. The measured energy bands confirm the presence of a Fermi surface. The oscillatory component of the magnetic susceptibility de Hass-van Alphen (dHvA) effect also confirm the presence of Fermi surface in its normal phase at low temperatures.

A small oxygen isotope shift had been found in Y-Ba-Cu-O. The very small oxygen isotope shift observed in 123 was taken to indicate that pairing of the charge carriers in this system is not phonon mediated. However, the substantial oxygen isotope shift obtained in the partial replacement of Y by Pr and Ca doped samples is consistent with pairing by high-frequency phonons, suggesting that modes involving oxygen motion are important in the mechanism responsible for high-T_C superconductivity (HTSC).

A quantitative surprise is the high ratio of the zero temperature gap to T_C, 2Δ (O) / $k_B T_C = 8$, obtained through photoemission experiments. They are consistent with tunneling, reflectivity or the knight shift measurements. Cuprate superconductors are of type II (λ / ξ » 1) and are in the clean limit. Large anisotropy of coherence lengths and energy gaps indicates weak correlation between Cu-O planes in the unit cell.

The paraconductivity analyses in the doped and undoped YBCO systems showed the 2D to 3D crossover when the system enters from high temperature to the mean field regime. The Anderson-Zou fit to the data is found to work well. There are results confirming the absence of appreciable pseudogap effects on the in-plane resistivity in optimally doped $YBa_2Cu_3O_{7-\delta}$ superconductors. The surprising manifestation of collective quantum effects in single-particle excitation spectrum may indicate that the pairing of electrons in the superconducting state cannot be reconciled with more conventional theories.

It has been theoretically predicted that the interaction between the two adjacent CuO_2 layers in $Bi_2Sr_2CaCu_2O_{8+\delta}$ would result in a doubling in the number of bands. The experimental confirmation of this bilayer splitting demonstrated that the interaction between neighboring CuO_2 planes strongly affects the electronic structure and suggest that the theories should include the bilayer interaction. Spin-charge separation is an exotic phenomenon in which the charge and spin of an electron are separated and behave like independent particles. There are experimental evidences of spin-charge separation in doped Cu-O chain.

The doped charge carriers in $Nd_{2-x}Ce_xCuO_4$ are electrons as opposed to holes for YBCO, BSCCO and the vast majority of HTSCs. It is now widely accepted that the superconducting pairing in the hole-doped materials is strongly dependent on the momentum of the electrons (d wave symmetry). It has been long believed that the pairing in the electron-doped materials had no such momentum dependence (S wave symmetry). However, the photoemission data detect the small but clear momentum dependence in the superconducting pairing demonstrates that the electron and hole doped materials may not be as disparate as originally believed, moving us closer towards a unified picture of the HTSCs.

The observed BCS like Bogoliubov quasiparticles in high Tc cuprate $Bi_2Sr_2Ca_2Cu_3O_{10}$ by ARPES studies support the BCS like theories. The observation of a Fermi edge along with many band structure-like features in angle resolved photoemission experiments have led to some support for a Fermi-liquid description. On the other hand, many of the normal-state properties, such as, the $\rho(T)$, the thermal conductivity K (T), the optical conductivity $\sigma(\omega)$, the Raman scattering intensity $s(\omega)$, tunneling conductance g(v), the nuclear relaxation rate $T_1^{-1}(T)$, small isotope effect, and the Hall coefficient $R_H(T)$ are all anomalous and are unlike those observed in any other metal or expected for a Fermi-liquid. The superconducting-state in the cuprates is rather un-remarkable, that is, the major new features are the high-T_C, the absence of coherence peak in T_1^{-1} near T_C and the high value of $2\Delta(O) / k_BT_C \approx 8$.

The mechanism for superconductivity should follow relatively easily once the much harder problem of the normal-state is worked out. At present no theory can account for all the normal phase data. So far, it is not possible to calculate with confidence the T_C of a particular model. One does not even know with certainty whether its ground state is that of normal-state, antiferromagnetic insulator, charge density Peierls insulator, or a superconductor.

The main issues cited as responsible for the failure of Fermi-liquid theory are: The low dimensionality, the close proximity of superconducting phase with a long range magnetically ordered AFM phase, the small carrier concentration number, the high $T_{C,}$ the high dominant wave vectors and frequencies, the strong coulomb interactions, the small isotope effect, the frequency dependence of relaxation rate, the controversial existence of the energy gap and the failure of the sum rules for the photoemission data.

Using the concentration of mobile holes in the CuO_2 planes the T_C for these materials has been estimated from the strong-coupling theory to be less than 30 K for the electron-phonon coupling constant $\lambda \rightarrow \infty$. This, suggest that the conventional mechanism of pairing via electron-phonon interaction will not do. Thus, the alternative proposed theories are : The Resonating Valence Bond (RVB) theory and its various generalizations (Luttinger liquid and Gauge field theory), the spin bags theory, the almost localized Fermi-liquid theory, the almost magnetic Fermi-liquid theory, the marginal Fermi-liquid theory, exciton mechanism, nested Fermi-liquid scheme, magnon and plasmon pairing mechanisms, bipolaron, soliton and bisoliton mechanisms, generalized BCS pairing theory, etc.

An ultimate microscopic theory of the high-*T*c superconductors may emerge after clarifying how the Mott transition and its proximity, namely the mother transition of many other competing orders, is so special in these materials. The difficulty over these past twenty years partly comes from the lack of good experimental probes for dynamical and short-range density (charge) correlations, although some signatures of static density fluctuations have been observed in STM. In contrast to magnetic correlations studied by neutron scattering and NMR, probes for wave number and frequency dependent charge correlations, such as, electron energy-loss spectroscopy or X-ray spectroscopy are still too poor to reveal the strong but diffusive charge fluctuations expected in the Mott proximity. A breakthrough of the resolution in such experimental probes may solve the long-standing puzzle.

The problem of HTSC is in fact a set of problems related to the unusual phases, phase transitions and crossovers in a quasi-two-dimensional doped Mott insulator. These materials challenge three basic paradigms of 20th-century solid-state physics: band theory, Landau's Fermi liquid theory and the BCS theory of superconductivity. This, together with the absence of small parameters, has made the progress on high-*T*c theory difficult.

CONCLUSION/RECOMMENDATION AND FUTURE WORK

If there is indeed a correlation between instability and the high-T_C, one might expect that as one continues to raise the T_C the instabilities will become so pronounced that exceptional synthesis procedures will be required. This is a considerable challenge for those attempting to raise the T_C. The materials are so complex that no theory can yet reliably predict the behavior of the new materials. The trick is to employ materials science, solid-state chemistry, intuition and hard work to find the right combination of elements to drive the T_C higher.

The field of high-*T*c superconductivity forces us to unify such concepts as superconductivity, antiferromagnetism, Hubbard subbands, and correlated electron states. One or possibly a small set of closely related approaches may fully explain high-T_C, as BCS did for low-T_C.

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