“A Snapshot View of High Temperature Superconductivity 2002”

Ivan K. Schuller[1], Arun Bansil[2], Dimitri N. Basov[1], Malcolm R. Beasley[3], Juan C. Campuzano[4], Jules P. Carbotte[5], Robert J. Cava[6], George Crabtree[4], Robert C. Dynes[1], Douglas Finnemore[7], Theodore H. Geballe[3], Kenneth Gray[4], Laura H. Greene[8], Bruce N. Harmon[7], David C. Larbalestier[9], Donald Liebenberg[10], M. Brian Maple[1], William T. Oosterhuis[10], Douglas J. Scalapino[11], Sunil K. Sinha[1], Zhixun Shen[3], James L. Smith[12], Jerry Smith[10], John Tranquada[13], Dale J. van Harlingen[8], David Welch[13]

[1]University of California, San Diego, [2]Northeastern University, [3]Stanford University,[4]Argonne National Laboratory, [5]McMaster University, [6]Princeton University, [7]Ames Laboratory, [8]University of Illinois, [9]University of Wisconsin, [10]U.S. Department of Energy, [11]University of California, Santa Barbara, [12]Los Alamos National Laboratory, [13]Brookhaven National Laboratory

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I. Summary

This report outlines the conclusions of a workshop on High Temperature Superconductivity held April 5-8, 2002 in San Diego. The purpose of this report is to outline and highlight some outstanding and interesting issues in the field of High Temperature Superconductivity. The range of activities and new ideas that arose within the context of High Temperature Superconductors is so vast and extensive that it is impossible to summarize it in a brief document. Thus this report does not pretend to be all-inclusive and cover all areas of activity. It is a restricted snapshot and it only presents a few viewpoints. The complexity and difficulties with high temperature superconductivity is well illustrated by the Buddhist parable of the blind men trying to describe "experimentally" an elephant. These very same facts clearly illustrate that this is an extremely active field, with many unanswered questions, and with a great future potential for discoveries and progress in many (sometimes unpredictable) directions.

It is very important to stress that independently of any current or future applications, this is a very important area of basic research.

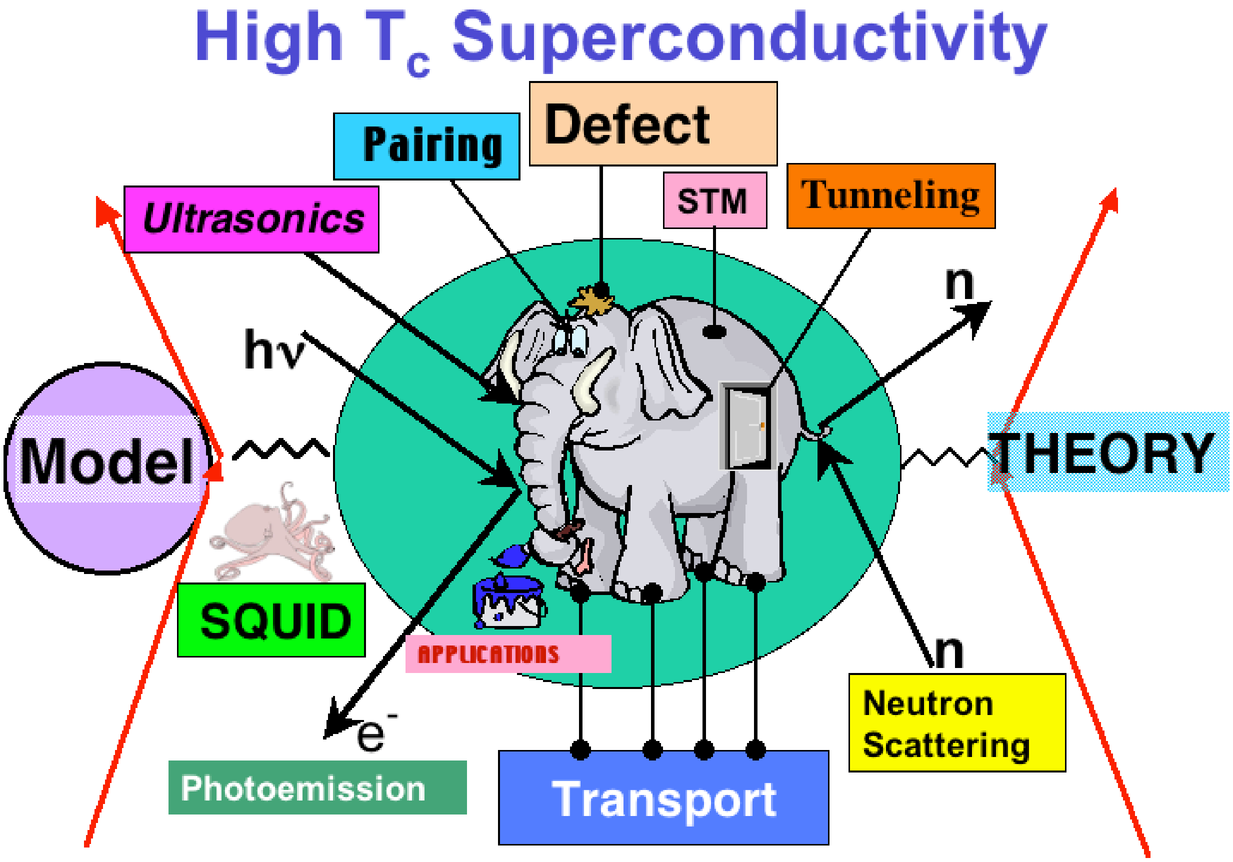

Fig. 1 Status of High Temperature Superconductivity.[1]

Basic research in high temperature superconductivity, because the complexity of the materials, brings together expertise from materials scientists, physicists and chemists, experimentalists and theorists. Much of the research in High T_c superconductivity has spilled over to other areas of research where complex materials play an important role such as magnetism in the manganites, complex oxides, two and one dimensional magnets, etc. Applications could greatly benefit from the discovery of new superconductors which are more robust and allow easier manufacturing. Perhaps this is not possible since a naive inspection of superconductors seems to indicate that the higher the T_c the more complex the material. An excellent review where many target needs for applications have been outlined is an NSF report of ~5 years ago. Many of the comments made there regarding applied needs, are still valid[2].

It is important to realize that this field is based on complex materials and because of this materials science issues are crucial. Microstructures, crystallinity, phase variations, nonequilibrium phases, and overall structural issues play a crucial role and can strongly affect the physical properties of the materials. Moreover, it seems that to date there are no clear-cut directions for searches for new superconducting phases, as shown by the serendipitous discovery of superconductivity in MgB_2. Thus studies in which the nature of chemical bonding and how this arises in existing superconductors may prove to be fruitful. Of course, "enlightened" empirical searches either guided by chemical and materials intuition or systematic searches using well-defined strategies may prove to be fruitful. It is interesting to note that while empirical searches in the oxides, gave rise to many superconducting systems, similar (probable?) searches after the discovery of superconductivity in MgB_2 have not uncovered any new superconductors. Anyhow, this illustrates that superconductivity is pervasive in many systems and thus future work should not be restricted to a particular type of materials systems. See Chapter II.

Research in the electronic properties of High T_c superconductors has proven to be particularly fruitful. This has lead to improvements in electronic structure techniques which unquestionably have an effect on other fields. The improvement on real and reciprocal space resolution uncovered many interesting properties. However, it is not clear at the present time whether many of these properties are related in some essential way to superconductivity or they are just accidentally present. It seems that the presence of competing phenomena is present in most high temperature superconductors. Thus it is natural to investigate systems which are close to some form of instability such as the metal-insulator transition, magnetic phases, electronic instabilities such as stripe phases, etc. Comparisons of classical infrared spectroscopy, and photoemission measurements with tunneling may prove to be fruitful. In particular, mapping with high resolution (in real and reciprocal space) the electronic structure may prove to hold some of the keys to the mechanism of superconductivity. To make these useful, issues such as surface contamination, surface segregation, and in general heterogeneity of the materials close to surfaces or interfaces must be addressed, and are particularly important in these very short coherence length superconductors. This is particularly important for surface sensitive probes such as photoemission. Several techniques such as Raman scattering, NMR and muon spin depolarization are not addressed in this snapshot, although they give valuable information and are heavily researched. Complementary measurements are particularly useful if a whole battery of tests, **in the same sample**, which are structurally characterized in detail, are performed. The "quality" of samples on the other hand, must be well established by structural criteria which are well defined "a-priori" and not based on circular or theoretical arguments. See Chapter III.

The properties of High Temperature Superconductors in a magnetic field have proven to be particularly interesting. A myriad of new phases have been uncovered in the vortex system and have lead to the establishment of a very complex phase diagram the details of which are still being established. The presence of many phases and the interaction/competition/closeness to magnetic phases allows for much new research using artificially structured pinning. New lithography and preparation techniques allow modifications and confinement of these materials in length scales approaching the superconducting coherence length and certainly the penetration depth. Moreover, novel imaging techniques are arising which can give detailed microscopic images of the vortex system. This of course can provide the microscopic picture of the magnetic state of high temperature superconductors and will probably also help improvements on their use. See Chapter IV.

Many basic research studies and a large number of applications require the High Temperature Superconductors to be in proximity with other materials. Thus issues of proximity effects, spatial variations close to an interface or surface, structural and materials variations are particularly important in thin film and/or nanoscopic structures. For this purpose it is important to investigate the mutual interaction between superconductors and other materials. This requires careful preparation and detailed characterization of inhomogeneous materials, together with superconducting measurements as a function of well-defined structural parameters. This may also allow addressing issues such as the importance of the proximity to other ordered phases such as magnetic and electronic inhomogeneities which are naturally existent or are artificially engineered. It is not even clear in the various models of high temperature superconductivity or even experimentally how the proximity effect occurs. What is the dependence of the order parameter in an ordinary or magnetic metal, or a low temperature superconductor when in proximity with a d-wave superconductor? See Chapter V

Contrary to low temperature superconductors, high T_c ones have received very little attention under nonequilibrium (time dependent, strongly driven, exposed to varying radiations, etc.) conditions. This may prove to be a very interesting and novel direction for ceramic oxides. These types of studies may hold important clues to the mechanism of superconductivity, may unravel new physics and are important in many applications. For instance, simple issues such as the microscopic nature or even existence of critical slowing down close to the superconducting phase transition has not been firmly established. See Chapter VI.

The theory of high temperature superconductivity has proven to be elusive to date. This is probably as much caused by the fact that in these complex materials it is very hard to establish uniquely even the experimental phenomenology, as well as by the evolution of many competing models, which seem to address only particular aspects of the problem. The Indian story[1] of the blind men trying to characterize the main properties of an elephant by touching various parts of its body seems to be particularly relevant. It is not even clear whether there is a single theory of superconductivity or whether various mechanisms are possible. Thus it is impossible to summarize, or even give a complete general overview of all theories of superconductivity and because of this, this report will be very limited in its theoretical scope. The general view point (determined by "majority vote") seems to be that low temperature superconductors are phonon mediated whereas high T_c ones are somehow "unconventional" and anisotropic, although the origin of the anisotropy remains controversial. Because of this, numerical studies in well-defined theoretical models may prove to be particularly illuminating and may help uncover the essence of superconductivity. Particularly, understanding and further developing the t-J model looks like a promising numerical direction. Electronic structure calculations combined with well developed methodologies seem to explain quantitatively many aspects of superconductors with moderate T_cs. How far can these type of approaches be pushed? Could they in fact explain ab-initio superconductivity in some of the cuprates? Moreover, first principle electronic calculations may be very useful in providing parameters for model hamiltonians. Another approach which at least allows parametrizing in some useful way the properties of superconductors has also been used. How far can these type of models go and how universally can they explain the (superconducting or normal) properties is not clear at this stage. There are several important issues which must be kept in mind. It may be that there is a theoretical model which has the essence of the problem in it and it either has not yet been developed or has not yet percolated to the conscience of the community. Moreover, it seems that to date no theory has been developed which has predictive power as far as materials system are concerned. Since purely theoretical approaches have difficulties so far in identifying a clear avenue for search, empirical studies in which materials parameters and properties are correlated with superconducting properties may prove useful[3]. This may serve at a later stage as a test ground for theories. Comparisons of theoretical ideas which rely only on the layered material of high T_c ceramics, with artificially engineered layered superlattices should not be neglected and may prove to be useful. See Chapter VII.

Finally, there seems to be still much work needed to understand in detail the connections, control and effect of defects on high temperature superconductivity. This of course is very important for applications, particularly those which require high critical currents such as power applications. Moreover, the intrinsic brittleness highlights that understanding and controlling the mechanical properties while not directly related to superconductivity, is a very important and promising new area of research, especially in connections with large scale applications. See Chapter VIII.

In the rest of this paper we will expand on these issues and attempt to outline some well defined promising directions of research. The focus is mostly on basic research challenges and opportunities, which hold back progress.

II. Structure, Bonding and New Systems

The discovery of new superconducting materials has played an important role in the advancement of the field of superconductivity research since its inception[4-7]. This was perhaps most dramatically displayed by the discovery of the high T_c cuprates in 1986. The influence of new superconducting systems continues to this day, for example through the discovery in 2001[8] of MgB_2. Thus far, the existence of a totally new superconductor has proven impossible to predict from first principles. Therefore their discovery has been based largely on empirical approaches, intuition, and even serendipity. This unpredictability is at the root of the excitement that the condensed matter community displays at the discovery of a new material that is superconducting at high temperature. New systems can be found by either bulk methods or thin film methods, each of which has its own advantages, disadvantages, challenges and opportunities. The search for new materials has always been[9], and remains an important area of research in the field of superconductivity.

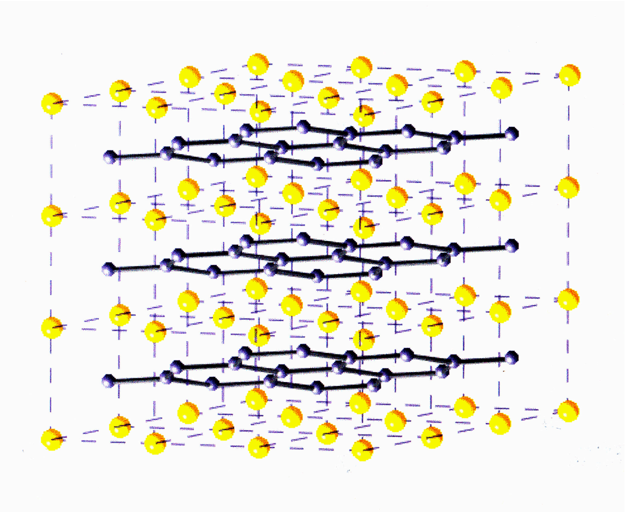

Fig. 2 The crystal structure of MgB_2. The graphite-like array of boron (shown in black) is critical to the occurrence of high temperature superconductivity in this compound.

Also important for the development of potentially practical materials and the understanding of the complex physical phenomena which occur in superconducting materials has been the use of chemical doping or manipulation to influence the electronic and magnetic properties of the superconducting systems. An example of the former chemical doping is the introduction of small flux pinning chemical precipitates in conventional intermetallic superconductors and 123-type superconductors. Examples of the latter are found in the "lightly doped" cuprates and other perovskite structure transition metal oxides where the concepts of charge and orbital ordering have recently emerged as important considerations in attempts to understand magnetic and electronic properties. These cooperative states join other such states such as charge density waves and spin density waves as critically influential in determining the ultimate electronic ground state of complex materials. Chemical doping has played an essential role in these areas. Importantly, it allows for the systematic variation of electronic properties as a function of variables such as lattice size, carrier concentration, and magnetic or non-magnetic disorder, providing a basis for the development of theoretical models. This area of research is highly active in the field of superconductivity, and will continue to be of great importance in the future.

1. Synthesis and Fabrication

a) Bulk

In the high density of states conventional intermetallic superconductors, the BCS coupling through the lattice may be viewed as a general lattice phenomenon. In more recently discovered superconductors, such as MgB_2, it has been found that one particular phonon mode – an in-plane boron mode that modulates bond lengths and angles within the flat B honeycomb lattice in the case of MgB_2 - is responsible for coupling to the conduction electrons and is the driving force for superconductivity[10, 11]. Conclusions about the nature of the phonons and electrons that are responsible for the superconductivity in a particular material can be arrived at nowadays by sophisticated experimental study and theoretical analysis. In particular the band-structure experts can calculate the effect that a particular phonon has on the electrons at the Fermi energy in a particular superconductor by doing “frozen phonon calculations”. Such calculations are highly instructive for superconducting materials like MgB_2.

This analysis is after the fact, unfortunately, for people whose interest is in finding the new superconductors in the first place. So given the fact that undirected combinatorial chemistry will never get through all the possible element/treatment combinations in a search for superconducting materials, one important issue to be resolved in future research is to translate the physics of superconductivity into a set of chemical hypotheses to guide the search for new ones. The era of finding new high temperature superconductors in intermetallic compounds like Nb_3Ge appears to be long gone. The new breed of high T_c superconductors is quite different - even beyond the cuprates, which are their own special case. The difference lies in the type of chemical bonding these superconductors display, even in what look like classic intermetallic compounds such as MgB_2 and $LuNi_2B_2C$[12]. Thus one important issue for future research is to explore how the nature of the chemical bonding present influences the superconductivity in “conventional” intermetallic compounds.

Initially promising reports of electronic doping through charge injection into a variety of organic and inorganic compounds in FET device structures have recently been called into question[13]. Nonetheless, conceptually they point out that another area of future research in new superconducting systems should be that non-thermodynamic synthetic methods should be actively pursued. Modulation doping, the chemical analogue of charge injection, for transferring charge between layers in fine scaled multilayerd films, has potential which is yet to be exploited. Other methods for non-thermodynamic synthesis with high potential for success include quenching from high pressure or from the vapor, epitaxial thin film layer by layer or block-by-block growth, photodoping, electrochemical synthesis at low temperatures, ion exchange, framework stabilization of structures, and electrochemical intercalation.

b) Thin Films.

There are many examples of stabilization of non thermodynamic compounds in thin films in both the cuprate superconductors and in dielectric or ferroelectric materials by using epitaxy with substrate or buffer layers. In the most extreme examples of this type of metastable material it may be a single atomic layer or even an interface that has the desired properties. On such short length scales, chemical bonding is the predominant influencing factor. Different physical and chemical methods of growth influence the behavior of surfaces and very thin layers. Great progress has been made in characterization after growth – such as Transmission Electron Microscopy (TEM) and X-ray probes, but a great deal more may be gained in the future by incorporating techniques that can be used *in situ* to characterize surfaces during growth.

Of particular interest in the search for new materials is the "phase spread method" used with success by some materials physicists. In this method, thin films are made by intentionally introducing composition gradients, for example by having three atomic sources in a triangular geometry, such that their deposition areas only partially overlap. The film thus fabricated contains mixtures of the source atoms in systematically varying ratios depending on proximity of substrate to one or another of the source. Annealing of such composition spreads under different conditions can be employed to search significant areas of phase space.

Photoexcitation provides another non-thermodynamic method to perform doping studies on thin films in a reproducible way without changing material, thus avoiding the inherent difficulties with controlling stoichiometry, uniformity, and homogeneity of the samples[14, 15]. Persistent photoexcitation has been performed in many cuprate superconductors and on the magnetic manganites at low temperatures below 100K. Large changes in conductivity, Hall effect, mobility, and superconducting transition temperatures have been observed. In the best model for this process, light generates an electron hole pair and the electron is trapped in a defect thus changing the hole doping in the electronically active layer providing a potentially useful way to trim device properties and "write" artificial nanostructures without need for lithography.

c) Doping in the Cuprate Superconductors.

The properties of the cation-substituted and oxygen-doped high-temperature superconductors have been studied in detail since 1987. In general, the physical properties (temperature-dependent resistivity, superconducting transition temperature, Hall effect, etc.) and the structural properties of the HTS cuprates behave quite differently as a function of substitutions in comparison to conventional superconductors. Doping and ion-induced disorder have shown that a small change in physical structure can induce a dramatic change in the electronic structure in these materials. This was one of the first indications that they were unconventional superconductors. The details of the effects of atomic substitutions or doping are not yet fully understood in the cuprate superconductors, and this represents an active area of current research. Concentrating on $YBa_2Cu_3O_{7-\delta}$ (YBCO) for example, some of these issues are:

i) Doping on the Y-site.

Doping with the heavy Rare Earth (RE) ions on the Y-site, even with Gd, does not affect T_c, except for substitutions of the Y with Pr. The effects of Pr-doping remain controversial.

ii) Doping on the CuO chains.

Substitutions of 3+ ions (e.g., Al, Co, Fe) primarily replace Cu in the CuO chains. Extra oxygen is simultaneously incorporated into the chain layer, the c-axis lattice constant increases, and an orthorhombic to tetragonal transition occurs. Since the extra oxygen compensates for the valence of the substituted cation, it remains an open question as to whether the resulting doped materials are underdoped or overdoped. Also, it has long been known that not only is the T_c of YBCO dependent on the oxygen concentration, but also on how the oxygen is ordered. Open issues remain, such as why do the chain oxygens need to be ordered to maximize the T_c?

iii) Doping in the CuO_2 planes.

Both Ni and Zn predominately replace copper in the CuO_2 planes without significant structural change. However, T_c falls faster in these cases than it does with increased 3+-cation doping on the chains or oxygen doping on the chains. That is an indication that the loss of structural continuity of the CuO_2 plane is more detrimental to the superconducting transition temperature than the lattice changes that occur due to doping on the CuO chains. There are interesting data comparing the Ni and Zn-doping: Tc falls faster with increasing the Zn doping than with increasing the Ni doping. Conversely, the room temperature resistivity increases faster and the Relative Resistance Ratio (RRR) [R(300) / R(0)-extrapolated] reduces faster with increasing Ni doping than increasing Zn doping. Therefore, Zn destroys the superconducting phase faster and the Ni destroys the normal metal phase faster. Remaining issues are: Why do Ni and Zn substitution reduce T_c so dramatically? and Why does Zn suppress the superconducting state faster than Ni, while Ni suppresses the normal state faster than Zn?

iv) The Role of the Charge Reservoir Layers.

The cuprates containing Hg, Tl and Bi ions in their charge reservoir layers have unusually high T_cs. These ions are known to charge disproportionate, which makes them negative U-centers. Under some circumstances it is known that negative U-centers can be superconducting pairing centers. It is of great interest to determine whether superconducting pairing on the charge reservoir layers is responsible for the enhanced T_cs of the Hg, Bi and Tl cuprates, and if so whether the negative U approach can be turned into a general method for finding and enhancing superconductivity.

2. Other Topics of Interest

a) Applied Pressure.

The investigation of high temperature superconductors under high pressure has the advantage that the basic interactions responsible for superconductivity can be changed without introducing disorder into the system as encountered in alloying experiments. The drawback is that one has to deal with massive high pressure cells, small sample sizes, and technical difficulties that increase with the higher the pressure range of interest. Measurements of the pressure dependence of T_c are the most straightforward since this can be accomplished through measurements of the electrical resistivity and the ac magnetic susceptibility under pressure. The electrical resistivity in the normal state, which can be accessed even below T_c by suppressing superconductivity with a magnetic field, yields complimentary information about phonons and magnetic excitations that are responsible for the superconductivity. Other types of measurements such as NMR and specific heat have been made under pressure. It would be useful to develop techniques for making other types of measurements under pressure and extending the range of pressures currently accessible.

b) Spin, Lattice, and Charge Correlations.

“Doping” generally refers to the introduction of charge carriers into the conduction or valence bands of a material. However, because of the large coupling between charge, spin and lattice in the cuprate superconductors and other transition metal oxides, doping of these materials with charge carriers can also be accompanied by the formation of static and dynamic spin and/or charge ordered phases on a microscopic scale. These "stripe phases," have recently been observed in many perovskite based transition metal oxides, including several cuprates, and may be a general feature of transition metal oxides[16, 17]. The role these microscopic inhomogeneous spin or charge phases play in high temperature superconductivity, magnetism, and other effects that have been attributed to them, is, however, unclear at this time.

The comprehensive understanding of spin/charge self-organization in oxides is a challenging task. This is a new viewpoint in the survey of strongly correlated phenomena in solids – a field that until recently has been primarily focused on the properties of nominally homogeneous systems. Intrinsically inhomogeneous spin and charge systems in transition metal oxides call for both original theoretical approaches and for the development of novel experimental tools suitable to deliver important information. Existing experimental information on the electronic and lattice properties of stripes systems is incomplete and therefore many fundamental problems related to spin/charge ordered regime in solids remain unresolved.

3. Conclusion

We believe that the opportunities for new materials to greatly influence the future of superconductivity research remain large, both from the point of view of fundamental science and the development of practical superconducting materials. We believe that chemical doping, non-thermodynamic synthesis, the discovery of totally new materials, the investigation of strongly correlated charge and electronic systems, and the use of chemical principles to help answer questions about the nature of superconductivity are exciting areas for future research.

III. Electronic Structure and Quasiparticle Dynamics

High-T_c superconductivity is achieved when a moderate density of electrons or holes is introduced in antiferromagnetic (AF) Mott-Hubbard insulator hosts by chemical or field-effect doping. Gross features of the evolution of the electronic structure as doping progresses from Mott insulator to d-wave superconductor are known from the systematic transport, photoemission and optical studies[18-21]. The doping-driven phase diagram of high-T_c systems is exceptionally rich owing at least in part to the fact that at the verge of the metal-insulator transition boundary magnetic, electronic, lattice and orbital degrees of freedom are all characterized by similar energy scales. Optimally doped cuprates (having highest T_c for a given series) reveal a well-defined Fermi surface in close agreement with the results of the band structure calculations[22]. Nevertheless, the dynamics of charge carriers appears to be highly anomalous defying the grounding principles of the Fermi liquid theory. Numerous attempts to describe the electronic properties using strong coupling Eliashberg theory have been only partially successful[23-25]. Using this approach it became possible to find a consistent description of many of the features established through a combination of tunneling, photoemission, optical and neutron scattering measurements for YBCO and the Bi2212 families of materials. However, many other systems of cuprates fail to follow the same patterns[26, 27]. Moreover, because of the extremely strong inelastic scattering established for most high T_c superconductors the concept of strongly interacting quasiparticles underlying the Eliashberg formalism is in question.

Early on it became established that superconducting currents in cuprates are carried by *pairs* of holes or electrons similar to that of conventional BCS superconductors. However, a viable description of the pairing interaction is yet to be found. Numerous experimental results indicate that the process of the condensate formation in cuprates is much more complex than the BCS picture of a pairing instability of the Fermi gas. One example of a radical departure from the BCS scenario is that the opening of the superconducting gap in cuprates is preceded by the formation of a partial gap (pseudogap)[28]. There is still a debate as to whether this pseudogap is related to the superconductivity. The pseudogap appears to be strongly anisotropic around the Fermi surface mirroring the anisotropy of the superconducting gap. These observations prompted the “precursor to superconductivity” scenarios for the pseudogap. Within this view, the formation of pairs precedes the development of global phase coherence between paired states[29]. Observations of vortex-like excitations[30] as well as of finite superfluid stiffness[31] at $T>T_c$ are in accord with the preformed pairs hypothesis. The process of the superconducting condensate formation in high-T_c cuprates also appears to be notably different from the BCS scenario. In particular, the energy scales involved in the formation of the superconducting condensate are anomalously broad and exceeds the magnitude of the superconducting energy gap by more than one order of magnitude[32, 33]. These latter results inferred from optical spectroscopy are consistent with the view that the kinetic energy is lowered in the superconducting state. Similar conclusions also emerged from the detailed analysis of the photoemission spectra[34]. The electronic properties of the high T_c superconductors have been probed by several complementary techniques. These techniques have shown substantial technological improvements in part driven by the need for higher energy and k resolution. In addition there is a growing belief that these materials may have real space inhomogeneities and so that a high resolution real space probe is desirable. Among the techniques that have revealed substantial insight because of technical improvements, we discuss electron tunneling, angular resolved photoemission spectroscopy, and infrared spectroscopy.

1. Techniques

a) Electron Tunneling.

Electron tunneling (both quasiparticle and Josephson tunneling) has been a powerful technique to probe the excitation spectrum, the superfluid density and the pair wave function phase of conventional superconductors. With high T_c cuprates, the technique has been no less informative. Currently, much of our understanding of the order parameter symmetry has come from Josephson effect studies[35] and the non-BCS nature of the excitation spectrum that comes about from the symmetry has been clearly observed[36]. C-axis and a-b plane quasiparticle tunneling have illustrated the extreme anisotropy of these superconductors and shown that surfaces are very different with possible bound states due to the broken symmetry at the a-b interface[37]. Intrinsic c-axis tunneling[38] has attempted to address the relationship between the superconducting gap and the pseudo gap. The debate over whether the pseudogap and the gap are intrinsically coupled continues.

STM studies offer an important additional feature that has already yielded some surprises. STM quasiparticle tunneling has allowed both microscopy and spectroscopy with good energy resolution and the spatial resolution to study the gap parameter on a length scale smaller than the superconducting coherence length[39]. Some of the current thinking on the high T_c superconductors concludes that there are intrinsic inhomogenieties (especially in the underdoped limits) in the superconducting properties. Coupling the high energy resolution with the high spatial resolution, along with the recently developed superconducting STM[40] will allow direct spatial studies of the energy gap, bound states and the superfluid density. Recent investigations have illustrated the local effects of non-magnetic and magnetic impurities[41] in the high T_c materials and a background periodicity in the electronic density[42] (charge density wave or spin density wave?) which requires further investigation. It is not clear whether this periodicity in the electronic density is associated with the superconductivity in these materials. Finally, the combination of high resolution quasiparticle spectroscopy and Josephson probe will allow quantitative investigation of spatial variations of the order parameter and superfluid density around impurities, at interfaces and proximity junctions. In conventional superconductors these two quantities are related but with spatial inhomogeneities, it is no longer required. For the high T_c materials, some theoretical models require inhomogeneities that would result in the superfluid density having different behavior than the energy gap. This will allow us to address both fundamental issues and applications. For example, current studies show that a magnetic impurity does not suppress the energy gap[31]. It has been concluded that superconductivity is not affected but the superfluid density has not yet been investigated. In addition, much is still to be learned about the proximity effect at the interface between the high T_c materials and other metals. Tunneling will allow us to probe this interface.

b) Angular Resolved Photoemission Spectroscopy (ARPES).

ARPES experiments have contributed to our understanding of the electronic structure and superconducting properties by revealing the Fermi surface information,[43] and a large superconducting gap anisotropy that is consistent with d-wave pairing state.[44]

Recent improved resolution, both in energy and in $\underline{k}$ have resulted in unprecedented data which allow us to map the electronic dispersion curves (E vs. k) for bands below the Fermi level E_F [45, 46]. Angle resolved photoemission studies are now mapping the dispersion curves for several cuprates (and other perovskite oxides). As a result of the enhanced energy and k resolution, it has been demonstrated that in addition to E and $\underline{k}$, the linewidths ΔE (related to scattering rate $1/\tau$) and Δk (related to the inverse mean free path $\frac{1}{\ell}$) can also be determined. While mapping these quantities over an extensive phase space of E and k is still to be done, these measurements have revealed some very important insight already. Close to E_f an electron mass enhancement[47-49] (E vs. k measures the velocity and hence the effective mass m*) is observed in the dispersion curves which is both energy and temperature dependent. These measurements can be thought of as directly probing the self-energy of the carriers with all their dressings as a result of the interactions the carriers experience. In conventional superconductors, these interactions and mass enhancements are a result of the electron-phonon interaction; the mechanism responsible for superconductivity in the simple materials. Indeed, for many in the field it was the measurement of the strength of the electron-phonon interaction (via tunneling for example) which confirmed the phonon mechanism of superconductivity. The measurements of ARPES are being carried out in several laboratories in the U.S. and elsewhere and the mass renormalization effects are observed at several facilities and in several materials.

There is still disagreement as to some of the details of these measurements and to their interpretation[48, 50, 51]. Electron-phonon interactions, electron-spin interactions and electron-electron interactions have all been suggested and all result in enhanced mass due to the interactions. Temperature dependent studies also illustrate that these interactions are at low energy and result from strong interactions.

It is clear that mapping of these dispersion curves over a wider volume of the E-k phase space is important. It is especially critical with the high T_c cuprates because of the large electronic anisotropy of the materials. Furthermore, because of the symmetry of the order parameter, mapping of the self energy effects as a function of <u>k</u> around the Fermi surface is especially critical. If these observed renormalizations are the signature of the mechanism responsible for superconductivity in the high T_c materials, an extensive map of the electronic renormalized map will be valuable if the analogy with low T_c superconductors is relevant. In the case of low T_c materials the renormalized mass $m^{*} = m(1 + \square)$ where $\square$ =electron-phonon interaction averaged over the Fermi surface.

Current ARPES measurements could be determining <u>quantitatively</u> the strength of the interaction and the mechanism of superconductivity. As a final caveat, it must be remembered that both APRES and tunneling are surface probes.

In this connection, inelastic X-ray scattering (IXS), which is not sensitive to surfaces or defects, is a valuable probe of bulk states. For high momentum and energy transfers IXS directly measures the ground state momentum density of electrons, while spin density is measured in magnetic IXS scattering. with improved resolution that has been achieved with synchrotron light sources, IXS has revealed surprising electron correlation effects with simple metals and has been extended to study the electronic excitations of the present compound of high T_c superconductors. Its application to ceramic superconductors would be most worthwhile.[52, 53]

c) Infrared Spectroscopy.

Infrared (IR) and optical spectroscopy is ideally suited for the studies of superconductivity because of the ability of these techniques to probe such fundamental parameters as the energy gap and the super fluid density[54]. Notably, IR spectroscopy allows one to investigate the *anisotropy* in these parameters through measurements performed with the polarized light[55]. Because IR/optical information is representative of the bulk and measurements can be performed on the micro-crystals, these studies allow one to examine common patterns of a large variety of materials which may not be suitable for examination with other techniques. Optical techniques offer means to probe strong coupling effects in the response of quasiparticles. In this context IR, tunneling and ARPES results are complimentary to each other. It is therefore desirable to "map" renormalization effects using a combination of several spectroscopic methods. Charge- and spin-ordered states in solids can be conveniently examined through the analysis of the IR-active phonon modes. The latter circumstance is important for the investigation of self-organization effects which dominate the dynamics of charge carriers at least in under-doped cuprates.

IR measurements can be performed in high magnetic field. Present work in the use of IR in high field experiments is restricted to a few experiments but several groups are actively involved into adapting IR instrumentation for these challenging measurements. These studies promise to yield detailed information on dynamics of both pancake and Josephson vortices. More importantly, DC fields currently available in optical cryostats (up to 33 T) are sufficient to destroy superconductivity thus giving spectroscopic access to the *normal* state properties at $T<<T_c$. Transport measurements in strong magnetic field highlighted anomalies of the normal state in LaSrCuO (LSCO) series of cuprates[56]. Spectroscopic measurements will be instrumental in distinguishing between (conflicting) interpretations of these results and will also help to unravel generic trends of the normal state behavior at $T<<T_c$ between several classes of superconductors.

2. Magnetism, Competing Order, and Phonons

a) Magnetism and Spin Fluctuations.

As discussed earlier, superconductivity in the cuprates is achieved by doping holes or electrons into an antiferromagnetic-insulator state. The magnetism is essentially an electronic effect, as it results from strong Coulomb repulsion between pairs of conduction electrons on the same Cu atom, together with the Pauli exclusion principle. Considerable knowledge of antiferromagnetism (AF) and spin fluctuations in the cuprates[57, 58]. has been obtained experimentally using neutron scattering, nuclear magnetic resonance (NMR), and muon spin rotation (□SR) spectroscopy. The general significance of antiferromagnetic correlations and spin fluctuations in theoretical mechanisms of high-temperature superconductivity is motivated by this experimental work.

In hole-doped cuprates, 2% holes doped into the CuO_2 planes are generally sufficient to destroy AF long-range order, but a minimum of 5-6% are necessary to induce superconductivity. Considerable attention has been devoted to characterizing the evolution of the AF spin fluctuations with doping. The bandwidth of the magnetic excitations, ~300 meV in the ordered AF, appears to change relatively little with doping. In LSCO, the low-energy spin fluctuations become incommensurate as doping increases, with a characteristic wave vector displaced from that of the AF by an amount □. Similar incommensurability has been observed in YBCO, but additional features are the presence of a gap in the low-energy fluctuation spectrum followed by a commensurate "resonance" peak. The gap and peak energies both increase with hole concentration up to optimum doping, at which the resonance-peak energy is ~ 40 meV. Recent results on other families of superconducting cuprates indicate that the resonance peak is a common, although not universal, feature[59].

Electron doping has a weaker effect on the AF state, with a transition directly from AF order to superconductivity occurring at an electron concentration near 12%. Initial neutron measurements indicate that the AF spin fluctuations remain commensurate in the superconducting phase. Studies over a broad energy range are made challenging by the presence of crystal-field excitations from the rare-earth ions.

Progress in the characterization of spin fluctuations has been enabled by the development and improvement of techniques for growing large single crystals and by forming large-volume mosaics of small crystals. Neutron scattering studies of hole-doped cuprate systems other than LSCO and YBCO are in early stages, and considerable progress is likely in the next few years. Improvement in the homogeneity of large underdoped YBCO crystals would be helpful for some of the issues discussed below. The availability of sufficient access to appropriate neutron scattering facilities may also be a limiting factor.

b) Competing Orders.

A phenomenon known as "stripe" order has been observed by neutron and X-ray diffraction in several variants of the LSCO family[60, 61]. Spin-stripe order is indicated by the appearance of elastic magnetic superlattice peaks at the same incommensurate wave vectors at which the low-energy spin fluctuations occur. These are usually accompanied by the observation of another set of superlattice peaks split about fundamental Bragg points, indicative of charge-stripe order. The presence of stripe order is generally (although not always, as in the case of La_2CuO_{4+y}) associated with a reduction in the superconducting transition temperature. However, there is also a linear correlation between T_c and the incommensurability of the spin fluctuations in the absence of stripe order.

There is also some evidence of stripe correlations in $YBa_2Cu_3O_{6+x}$ O chains. The temperature dependence of the associated superlattice intensities suggests a coupling to electronic correlations, and possibly to charge stripes[62]. Certain spin fluctuations have been found to have an incommensurability similar to that found in LSCO; however, the cause of the incommensurability is controversial.

The recent scanning tunneling microscope (STM) observations of spatial modulations of the electronic density of states (DOS) in the CuO_2 planes of BSCCO has stimulated considerable speculation. The observed period of 4a (a, the in-plane lattice constant) suggests a connection with the charge and spin stripes found in LSCO. Clearly, a combination of tunneling and scattering studies is needed to clarify the nature of the modulations.

There are many unresolved issues associated with the problem of stripes. Is stripe order a type of electronic instability, like conventional charge-density-wave order, that only competes with and limits superconductivity? Is it possible for a stripe-liquid phase to exist? Are stripe correlations common to all superconducting cuprate families, or do they only occur in special cases? Are spin stripes always associated with charge stripes, or are these distinct types of order? Do stripes (or possibly another type of inhomogeneity) exist in electron-doped cuprates? Studies with a wide range of techniques will be needed to answer these questions. Stripes are but one kind of order that has been proposed to have a connection with the various "pseudogap" phenomena that are observed in underdoped cuprates[63]. A number of theories have put forward the hypothesis that a new order parameter appears in the pseudogap regime. Two particular examples are quadrupolar orbital currents , and the staggered flux phase or d-density-wave (DDW) state. In both cases, orbital currents result in local magnetic moments that should be, in principle, detectable by neutron scattering. So far, neutron scattering experiments have been unable to find evidence for such phases, which predict no breaking of translational symmetry; however, the presence of quadrupolar currents provides a possible explanation for the recent observation of time-reversal-symmetry breaking by photoemission[64]. The possible existence of orbital moments remains an open issue.

c) Phonons and Electron-Phonon Interactions.

The role of electron-phonon interactions in the cuprates has been the subject of renewed interest, motivated in part by a recent interpretation of ARPES data.[28] An important technique for characterizing phonon dispersions and densities of states is inelastic neutron scattering. (Note that neutron measurements of the phonon DOS in MgB_2 provided an important validation of the theoretical evaluations of electron-phonon coupling in that system.) Dispersion anomalies in the Cu-O bond-stretching modes, clearly associated with some kind of electron-phonon coupling, have been the subject of controversy for several years. The experiments are constrained by weak scattering cross sections and limited crystal size. Further experimental studies, together with serious theoretical analysis, are necessary in order to make real progress in this area. Inelastic X-ray scattering has also been used recently to study optical phonons in a cuprate.

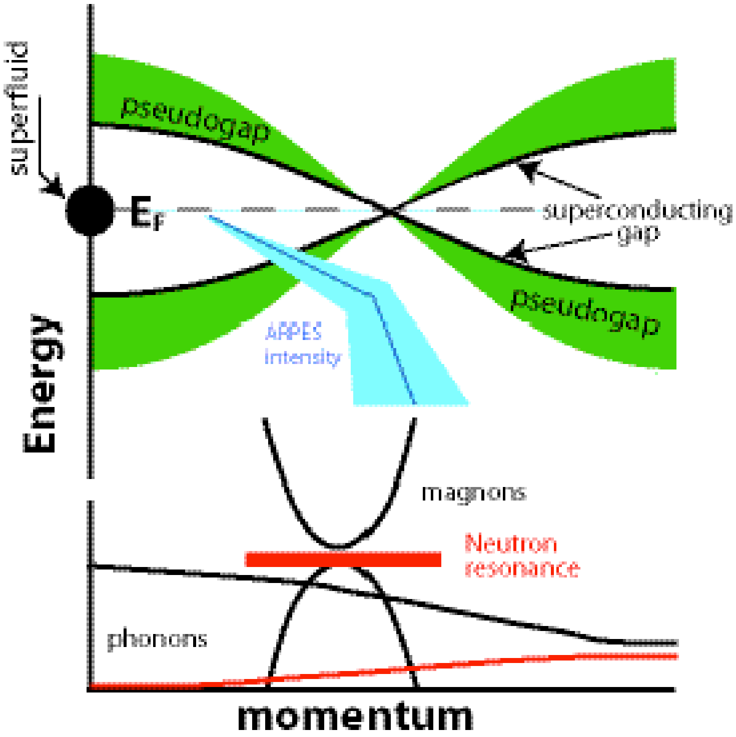

Figure 3. Schematic representation of excitations and collective modes in high-T_c superconductors. A remarkable variety of effects in these materials have typical energy scales of about 50-70 meV, including: phonons, magnetic resonance, superconducting gap and pseudogap as well as “kinks” in the ARPES spectra. Competition, interplay and interdependence between these effects are responsible for complexity of the strongly correlated state in these materials.

IV. Vortices

Most of the electromagnetic properties of Type II superconductors are determined by vortices in static and dynamic configurations. Rapid progress in manipulating and measuring vortices in recent years has greatly expanded the limits of known and imaginable vortex phenomena. This chapter outlines several research directions that are now within reach and that will develop new concepts and strategies for fundamental science and applications.

1. Single Vortex Physics.

a) Confinement.

Advances in micro- and nano-scale patterning and in high sensitivity measurements now enable studies of *single* vortices, allowing a wide range of new physics to be explored. Vortices enter mesoscopic samples[65-68] one-at-a-time at field intervals determined by flux quantization, $\Delta H \sim \Phi_0/L^2$ where Φ_0 is the flux quantum and L the sample dimension. The entry of each vortex produces a step change in the magnetization, corresponding to a *first order* phase transition. In circular disks, vortices are predicted to configure in shell patterns[69] reminiscent of electrons in atoms and leading to magic numbers of high stability. At certain fields a collection of discrete Abrikosov vortices transforms to a single *giant vortex* containing the same number of flux quanta and a circulating current at the outer edge of the sample. This phase transition is reminiscent of Wigner localization in electronic systems. In lower symmetry disks such as squares, vortices and antivortices coexist to simultaneously satisfy flux quantization and rotational symmetry[67].

Studies of confined vortices can be extended to layered superconductors such as $NbSe_2$ and the cuprates, where the superconducting coherence length ξ and the magnetic penetration depth λ are quite different, and to other experimental probes like STM that directly image the superconducting order parameter. Confinement need not be limited to a single disk. Arrays of disks, each containing confined vortices, can interact through a superconducting substrate. Confinement in a line geometry[65] allows *motion* of confined vortices to be studied[70]. Confined disks connected by lines offer many analogies to single electron behavior including the Coulomb blockade and single electron tunneling.

Individual vortices in an array can be manipulated by imposing an artificial mesoscopic template. One approach is to lithographically pattern a superconducting film with an array of holes, or antidots, each of which traps one or more vortices[71-74]. Trapping vortices one-by-one has practical implications: it can dramatically enhance the pinning effectiveness and critical current, and it can lead to extremely sharp switching effects at matching fields. These switching features offer the potential for three terminal devices, where the supercurrent across the antidot array is modulated by a control magnetic field operating near the matching field. Antidots are predicted to trap vortices with multiple flux quanta if the hole size is large compared to the coherence length. The properties of these multiquanta vortices are largely unexplored. Such antidots, for example, could enable the construction of information storage devices operating with integer rather than conventional binary bits.

Mesoscopic templating can be extended in several exciting directions. The technique can be applied to cuprate high temperature superconductors[75], where the nanoscale coherence length enables many tens of flux quanta to be trapped in a single mesoscopic hole. Unlike low T_c superconductors, the cuprates have clearly defined lattice, liquid, and glassy phases that will react quite differently to the imposed order of the template. First order vortex lattice melting, for example, is expected to be fundamentally modified by commensurate or incommensurate templates. Aperiodic templates provide another new direction. The vortices trapped in the holes create aperiodic scattering centers for free interstitial vortices whose dynamics will be quite different from those in ordered or random pinning arrays. Templates created to date have been limited by lithography to lattice spacings slightly less than one micron, putting the first matching field at about 20 Gauss. Electron beam and self-assembly techniques, for example based on diblock copolymers[76] anodic aluminum oxide[77] or inverse micelles[78], can be used to make templates with nanometer lattice constants. This much smaller spacing puts the commensurate vortex lattice in the strong interaction limit where collective effects dramatically alter its behavior. The one study on dense templates reported so far[79] shows that strong pinning persists well below T_c. High density templates bring the first matching field up to the kG range, much more interesting for applications than the tens of Gauss range accessible to lithographic templates. High density templates offer an intriguing new strategy for pinning the vortex liquid, where eliminating shear motion requires one pin site per vortex. In BSCCO and YBCO this opens large areas of the H-T phase diagram to practical use.

b) Pseudovortices and Vortex Core States.

The observation of unusual thermomagnetic effects in the underdoped region of LSCO above the superconducting transition temperature and below the pseudogap temperature[80] suggests that vortex-like excitations may be associated with the pseudogap state. The properties of these pseudovortices are still under examination and may hold important insights into the underdoped state. Pseudovortices may be observable as fluctuations using experiments with short time scales and local resolution, such as magnetic resonance or muon spin rotation.

The suppression of the superconducting energy gap in the vortex core creates a natural potential well that captures observable bound states in cuprate superconductors[81, 82]. These bound states provide a window on the nature of pairing, because they are sensitive to the presence of nodes in the gap that distort the core potential. STM sees not only the bound state, but also the anisotropy of the energy gap around the core, providing direct information on the nodal structure. These experiments would be particularly valuable if performed systematically for under and over doped regimes, where the nature of the normal and superconducting states changes continuously. In other organic and heavy fermion superconductors where the order parameter is a complex vector, the core states will display subtle details reflecting the exotic pairing. These core states are within reach experimentally but remain unexplored.

In the vortex core the superconducting order parameter is suppressed, providing a fascinating opportunity to search for competing types of order without physically altering the material. Indications of spin density waves[42] and pseudogaps[83] in the cores of BSCCO suggest a strong interplay of these types of order with superconductivity. The same approach could be employed to search for competition with antiferromagnetism[84] charge stripes, and other proposed ordered states.

The existence of two superconducting gaps[85] in MgB_2 raises fundamental questions about their effect on the core states. Strong variations in the core potential and the bound states are expected as the relative strength of the two gaps varies with temperature and field. This fascinating area is now within reach and is virtually unexplored.

c) *Hybrid Materials*.

We are now entering a new era of materials sophistication allowing studies of superconductors exposed to *internal* magnetic fields. Such internal fields arise in magnetic/superconducting hybrid structures[86], including naturally occurring $RuSr_2GdCu_2O_8$ [87] and the magnetic borocarbides[88, 89], and artificial hybrid structures containing patterned magnetic and superconducting layers[90]. There are fundamental questions regarding how superconductors respond to internal magnetic fields: the conventional mechanisms of Meissner shielding and vortex penetration for external fields are not necessarily adequate.

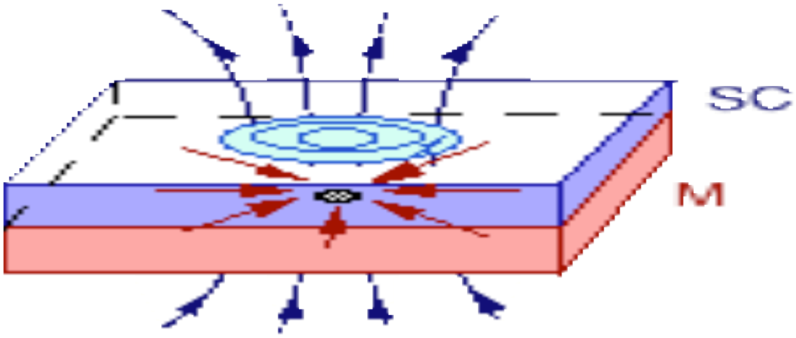

Fig 4. Superconductor/magnet bilayer. The vortex field polarizes the magnet locally, producing a radial magnetic texture.

In bilayer hybrids, the field of an individual vortex in the superconducting layer locally polarizes the adjacent magnetic layer creating a tiny *magnetic texture*.[91] Fig 4 shows a radial magnetic texture, where the vertical arrows represent the vortex magnetic field and the horizontal arrows the induced polarization of the magnetic layer. The coupled vortex-magnetic texture pair is a new compound object whose static and dynamic properties are virtually unexplored. One important element is the interaction between pairs, which is mediated by dipole and exchange interactions in the magnetic layer, Lorentz forces in the superconducting layer, and magnetostatic interactions between the layers. The resultant interaction potential is distinctively more complex than the simple repulsive potential of bare vortices. Dynamics brings in yet another element, the de-polarization and re-polarization of the magnetic layer that is required if a vortex in the superconducting layer is to move. Beyond the new physics of vortex-texture pairs, there is an additional attractive feature. The properties of the hybrid can be tuned by selecting the materials (e.g., the easy direction and the anisotropy in the magnetic layer), the relative thickness of the two layers, and the magnetic field direction. In multilayer hybrids with parallel applied field, an array of π-Josephson vortices can be formed, while tipping the field away from the layers induces Abrikosov-texture pairs.

There are equally fascinating possibilities in hybrids composed of magnetic dots deposited on a superconducting layer. Here the magnetic dot is a pin site that is isolated from the superconductor, avoiding deleterious effects of the pinning defect on current flow. Recent work on superconducting/magnetic dot hybrids[92-94] has defined several important issues, such as (i) the spontaneous creation of vortices and antivortices in zero applied field, (ii) the annihilation of antivortices by external field-generated vortices, (iii) the nature of matching field effects, (iv) the effect of magnetic dot repolarization at high field, and (v) the dynamics of dot-generated vortices under a driving Lorentz force. These basic unexplored issues become even more fascinating when the scale of the magnetic dot array is reduced from present day lithographic dimensions to much smaller self-assembled dimensions. The interaction of flexible and compressible vortex lattices with rigid pinning geometries has many analogies in epitaxial growth, absorption of noble gases on surfaces and even plasma physics in confined geometries. Thus progress in this area has broad relevance well beyond the field of superconductivity.

2. Multivortex Physics

a) Disordered Glassy and Liquid States.

The *collective behavior* of vortices is much like that of atoms: their mutual interaction energy creates lattices, quenched disorder by random pinning produces glasses, and thermal disorder melts the lattice or glass to a novel liquid state. The liquid and glassy states of vortex matter offer major challenges for understanding the magnetic properties of superconductors. Two kinds of glassy state have been proposed, the vortex glass[95] for disorder by point defects, and the Bose glass[96] for disorder by line defects. While experiments confirm the second order Bose glass melting transition, the tilt modulus and the resistive behavior of these disordered systems are at odds with each other and with theory[97]. For point disorder, even the voltage-current scaling behavior expected at melting is not observed[98] . Experimentally, lattice and glassy melting coexist in the same phase diagram[99-101], sometimes accompanied by novel “inverse melting” regions. Quasi crystals are another disordered phase of vortex matter, triggered by pentagonal or decagonal boundaries. The thermodynamics of melting in this phase intermediate between lattice and glass will be fascinating.

The vortex liquid shows equally fascinating behavior arising from *thermal* disorder rather than quenched disorder. Recent specific heat measurements[102] reveal two liquid phases separated by a second order phase transition. Understanding the nature of these two phases and the transition between them is a challenge not only for vortex matter but also other line liquids like polymers and liquid crystals. The vortex liquid offers another promising opportunity, to study the *interplay* of thermal and quenched disorder. The addition of quenched disorder to the liquid shifts the freezing transition up for columnar defects, down for point defects. The effect of the two kinds of quenched disorder on liquid state thermodynamics and on its driven dynamics is ripe for incisive experiments. Disordered vortices offer a rich complexity that is easily accessible experimentally yet so far defies theoretical description. Their behavior is fundamental to applications of superconductivity, and to the basic science of condensed matter systems generally.

b) Dynamic Phases.

The rich equilibrium phase diagram of vortices is matched by its driven dynamic behavior. The onset of motion at the critical current is a complex dynamic process governed by the distribution of pinning strengths, the vortex-vortex interactions, the temperature, and the driving Lorentz force. The plastic motion that normally accompanies depinning can now be directly observed through Lorentz microscopy[103] and magneto-optical imaging[104]. This emerging spatio-temporal resolution opens possibilities for systematic experimental studies to characterize the depinning process as a function of the basic variables. Such previously hidden onset phenomena as vortex channeling, vortex hopping from pin site to pin site, and the distinction between avalanche and continuous onset are becoming observable. This wealth of experimental information drives new theoretical descriptions of the depinning process. The plastic motion inherent in depinning makes its description in terms of partial differential equations of hydrodynamics challenging. However, statistical descriptions in terms of time dependent position and velocity correlation functions can be created that break new ground for describing the onset of plastic motion. Beyond depinning, there are a host of dynamic phenomena that are now amenable to observation, including vortex creep, thermally assisted flux flow, hysteresis in I-V curves, and memory effects. The concept of vortex *focusing* and *rectification* through the ratchet effect is especially interesting[105]. A fundamental microscopic understanding of these phenomena would lead to better engineered superconducting devices where stability and high depinning forces are crucial [106].

c) Josephson Vortices and Crossing Lattices.

Highly layered cuprates such as BSCCO support naturally occurring Josephson vortices, where the absence of a core and the large lateral penetration depth fundamentally alter the behavior typical of Abrikosov vortices. The two kinds of vortices co-exist and interact in the presence of a tilted applied field, where the perpendicular field induces a pancake vortex lattice and the parallel field induces a Josephson vortex lattice. The two *crossing lattices* interact to produce a complex phase diagram[107], containing spontaneous vortex stripes and intricate melting behavior for fields very close to the ab plane[108]. Advances in scanning Hall probe technology[109] and magneto-optical imaging[110] now allow these crossing lattice states to be imaged, directly illuminating these phase transitions in real space. The dynamic properties of Josephson lattices are also fascinating. Because they have no core and no conventional pinning, Josephson vortices can be driven at very high speeds. They are predicted to undergo a dynamic phase transition, from a highly distorted hexagonal structure at low speed to a stacked configuration at high speed[111]. The most remarkable prediction is that the high speed Josephson lattice emits Terahertz radiation with a frequency inversely proportional to the transit time for one lattice constant[112]. This offers the appealing possibility to create a new class of Terahertz radiation sources from dc components, with an adjustable frequency determined by the driving current and applied magnetic field.

3. Instrumentation.

Advances in STM, scanning Hall probes, magneto-optical imaging, Lorentz microscopy, high sensitivity specific heat and magnetization have driven recent and rapid progress in vortex physics. Further advances in instrumentation are on the horizon. Lorentz microscopy of vortex systems has recently been achieved at 1 MeV, showing unexpected changes in vortex orientation in BSCCO films[113] and dynamic structure in apparently static crossing lattices[114] Magneto-optical imaging can now see single vortices[104], opening a new window on real space dynamics. Higher resolution can be achieved with development of *near field* magneto-optical imaging, an advance that is within reach using available techniques. Specific heat experiments are ripe for much higher sensitivity using MEMS (micromachines) to eliminate addenda corrections and innovative temperature sensing. This new instrumentation will drive not only vortex physics but also will advance many other areas of condensed matter physics.

V. Proximity and Interface Effects

The superconducting proximity effect involves the mutual influence of neighboring superconducting and non-superconducting materials across an interface[115]. Such mutual influences can be profound. They can affect greatly the physical properties of both materials and are important in any application or scientific measurement that involves interfaces. Related effects occur at vacuum interfaces at the surface of a superconductor. The proximity effect is central to the physics of the coupling of superconductivity across non-superconducting barriers that make possible the Josephson junctions used in high-T_c superconducting electronics[116] and the grain boundary interfaces that are presently the primary factor limiting current flow in high-current superconducting tapes[117]. The proximity effect is also central to the broader application of the extremely powerful but surface sensitive techniques of photoemission spectroscopy and the growing arsenal of scanning local probes to these materials. The importance of grain boundaries as current liming factors in HTS tapes is also discussed in

Chapter VII of this report. And the importance of surface effects in the application of ARPES and scanning probes is discussed in Chapter III.

To all of this must be added the possibility of surface doping through the use of charge transfer from deposited over-layers or the electrostatic field effect. The recent determination of scientific misconduct in some reported results using field-effect doping to induce high-temperatures superconductivity does not undermine the basic scientific rationale for such work. Indeed, field effect doping (both capacitive[118] and ferrolectric[119]) has a long history that continues up to today. The situation has been reviewed recently[120]. Clearly, charge transfer and field-effect doping remain potentially elegant approaches to creating new superconductors and developing model systems for studying two-dimensional superconductivity.

For all these reasons mastery of the proximity and interface effects in the high temperature superconductors is essential to progress in the field.

In conventional, low-T_c superconductors the understanding of the proximity effect is relatively well developed for interfaces with normal metals[121]. The reasons are the power of BCS theory along with the simplification provided by the generally long superconducting coherence lengths typical of low-T_c materials (and conventional normal metals). These long coherence lengths tend to average out and temper interface effects and thereby permit the use of simple, phenomenological boundary conditions for most purposes. The proximity effect with a ferromagnet is qualitatively different, however, and its understanding remains under developed. The new twist here is that the pair wave function has an oscillatory decay in the ferromagnetic (FM) material[122], in contrast to the simple exponential decay found in the normal-metal case.

High-T_c superconductors are very different. The very short coherence lengths characteristic of these materials make them much more susceptible to the influence of neighboring materials and internal defects virtually at the atomic level. Hence, the use of phenomenological boundary conditions is problematic, and microscopic theory will have to play a larger role. Of course, there is no well developed microscopic theory of the high-T_c superconductors. In addition, the strong doping dependence of the cuprate superconductors makes them sensitive to charge transfer at interfaces, where there is a tendency to form npn-like junctions[123], introducing further new complexity. The d-wave nature of the pairing also leads to new features in the proximity effect (and the related Andreev scattering process at interfaces) that have not been fully explored. One now well-accepted example is the reduction of the pair wave function to zero at surfaces whose normal points along the direction of the nodes in the energy gap[124].

There are also intriguing experimental results that suggest new physics is operating in the proximity effect with the high-T_c superconductors. The anomalous normal state properties of the cuprates, particularly in the pseudo-gap regime at low doping, seems incompatible with the use of the conventional theory (based on low-T_c

superconductors and normal metallic behavior) to describe the proximity effect with these phases. In addition, various systematic studies of the proximity Josephson coupling of the ab-planes of the cuprate superconductors across these normal phases imply characteristic lengths of the proximity coupling that are larger than can be readily explained with conventional ideas[125]. The alternative possibility that longer coherence lengths are possible in the normal planes and/or that the range of the proximity effect with conventional normal metals on the c-axis of BSCCO is shorter than can be readily explained with conventional ideas[126] is intriguing.

From the theoretical perspective, understanding of the proximity effect with a material near a quantum phase transition (such as the superconductor/ insulator or metal/insulator transitions) with their associated quantum fluctuations is lacking even in the case of conventional superconductivity. It is presumably even more challenging in the case of the cuprates, which exhibit several such transitions as a function of doping, due to their highly correlated nature. In addition, there are speculations that negative U centers in the blocking layers are playing a role in the high-T_c of some cuprates in a kind of internal proximity effect[127].

Finally, the ability to exploit widely the powerful but inherently surface sensitive electronic probes of the high-T_c superconductors such as ARPES and the various emerging scanning probes will depend on dealing somehow with their complicated surface chemistry and altered doping of the CuO_2 planes near the surface due to the lack in general of a charge neutral cleavage plane in the unit cell of the cuprates, with the notable exception of $Bi_2Sr_2CaCu_2O_x$ (2212 BSCCO).

Key to understanding proximity and interface effects is the controlled preparation and characterization at the atomic level of the various interfaces of interest. Only by creating and understanding such model interfaces can the necessary phenomenology be developed that can guide applications (with their real, more complicated interfaces) and permit unambiguous scientific study of these materials with surface sensitive techniques.

Fortunately, recent advances in the controlled thin film deposition of highly refined interfaces of various kinds have been developed for the high-T_c superconductors and complex oxides more generally[128]. Atomic layer (or block by block) epitaxial growth has been achieved in some cases. Grading of individual layers as a film is built up may be necessary and likely is possible. The same techniques may also be useful in preparing the surfaces of bulk single crystals for study by ARPES and/or scanning probes.

The techniques capable of such refined interface preparation involve the combination of very well controlled deposition techniques with various *in-situ* means of monitoring the growth. These include Molecular Beam Epitaxy (MBE), Pulsed Laser Deposition (PLD) and sputtering. The need for an oxidizing atmosphere presents technical problems, but these are increasingly under control. *In-situ* Reflection High Energy Electron Diffraction (RHEED) is now commonly available for structural characterization and techniques to measure *in-situ* and in real time the temperature and composition of a growing film are likely to become available. Such instrumentation will greatly facilitate progress. *Ex-situ*, post-deposition characterization is necessary, however, in order to confirm the structure away from the growth conditions.

At the same time, techniques for preparing well-defined grain boundaries of various types for physical study in both crystals and thin films have been developed. Advances in electron microscopy have also been developed that permit not only the structural characterization of the grain boundaries but also determination of the spatial dependence of the electric potential (and therefore the distribution of charge) across the boundary, at least on average. Such information will greatly facilitate progress in understanding the electrical properties of these grain boundaries. Still needing development are probes capable of characterizing the lateral dependence of the structure and properties of these interfaces (particularly electrical transport). Presumably local scanning probes can be brought to bear usefully on these questions. Similarly, techniques need to be developed that can reveal the point defects present near the boundaries that are not visible in TEM and may be playing a significant role in achieving charge neutrality near the boundary.

In concert with better sample preparation and more thorough physical study will need to be the systematic development of phenomenological theories that incorporate appropriately the known physics of the high-T_c superconductors and the realities of the materials themselves. First principle predictive value is probably not possible nor is it necessary from the point of view of furthering the science. Phenomenological models may provide useful models of interfaces for applications and guide the empirical process of materials optimization.

In summary, study of the proximity effect is a critical element in the evolving study of the high temperature superconductors. The key issues are: developing the model materials systems that will enable understanding at the required atomic level; developing tools to make and measure such interfaces, in particular scanning probes; surface doping and charge transfer studies, developing a unified theory of the proximity effect that deals with the material realities and the novel physics of the high-T_c superconductors; and applying all this knowledge in surface sensitive studies of these materials.

VI. Nonequilibrium Effects

A very general case of nonequilibrium dynamics in an electronic system starts by creating a high-energy electron (e.g., by optical absorption) followed by a cascade of excited states with smaller and smaller energies until the excess energy can escape the system, generally by phonons. In superconductors, nonequilibrium effects also occur with a transport current, for example, at interfaces exhibiting proximity effects, including grain boundaries (see Chapters V and VIII). The nonequilibrium effects of currents are especially important when magnetic vortices appear either from applied fields or the self-field of the current. The excitation energies are not too large ($<k_BT_c$) in these cases, which are discussed in the dynamic phases of vortices part of Chapter IV and under pinning in Chapter VIII.

Returning to the cascade processes mentioned at the start, these are indicated schematically in Fig. 5. They include electron-phonon and electron-electron scattering and are relatively fast, being $\sim 10^{-12}$ sec to achieve thermal energies[129]. The eventual loss of excess energy results from the escape of phonons from a finite sized sample and it is much slower, being generally $\sim 10^{-6}$ sec, due to the small velocity of sound and significant phonon-electron scattering. In the case of a superconductor, this strongly affects the final relaxation step, the recombination into Cooper pairs and escape of the excess energy by phonons. In superconductors, scattering between electron-like and hole-like branches (see Fig. 5) only occurs after 'thermalization' to energy scales of order of the energy gap. In high-temperature superconductors (HTS), the d-wave energy gap depends on the momentum direction, exhibiting nodes along the (□, □) wave vectors. Thus a new element of nonequilibrium processes in HTS is the relaxation of momentum *around* the Fermi surface.

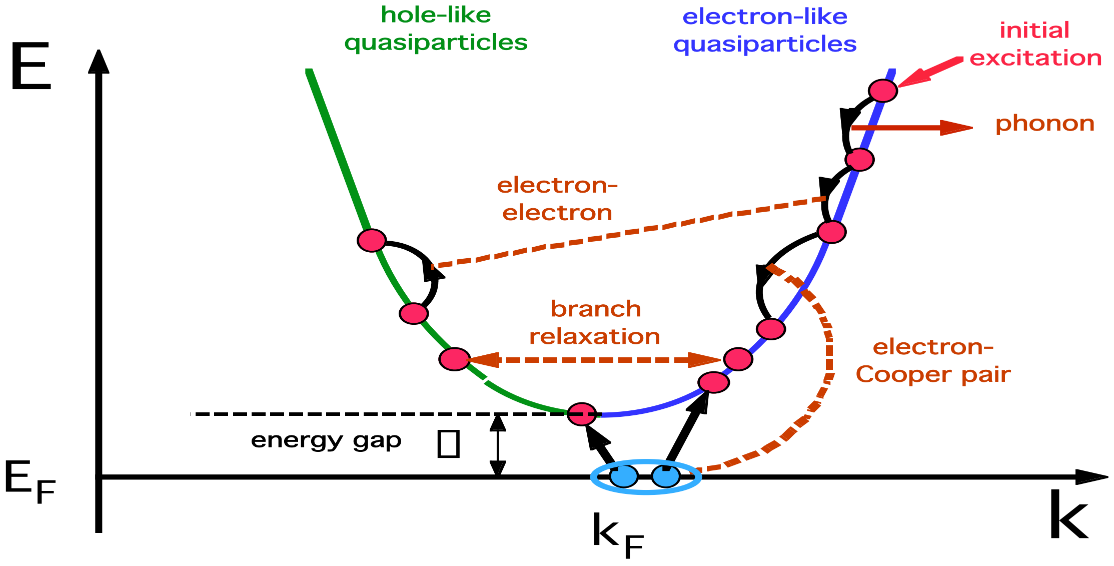

Fig. 5. Energy, E, versus momentum, k, for quasiparticle excitations in a superconductor with energy gap, □, showing electron-like ($k>k_F$) and hole-like ($k<k_F$) excitation branches. Also shown schematically are possible relaxation cascade processes for an initial electron-like excitation of energy, E>>□. Energy relaxation occurs by emission of a phonon, scattering off another quasiparticle or breaking a Cooper pair. Relaxation between the electron-like and hole-like branches occurs preferentially when E~□. The final step (not shown) is the relaxation of the excess quasiparticle density back to Cooper pairs and the concomitant escape of a phonon with energy ~2□.

Progress has been made to understand the fast scattering rates in HTS using thermal Hall conductivity[130], microwave absorption[131] and optical pump-probe experiments[132-136], but crucial pieces are missing. These include systematic studies that cover a wide spectrum of pump and probe frequencies, other complementary experiments and connections to theoretical predictions. Less attention has been paid to the traditional nonequilibrium studies[137, 138] in LTS that have addressed a wide range of effects of excess quasiparticle densities and/or branch imbalances between electron-like and hole-like quasiparticles. The opportunities in the latter case are exotic, numerous and largely untapped.

It is quite interesting that the scattering times derived from thermal conductivity[130], microwave absorption[131] and optical pump-probe experiments[132] exhibit a very similar magnitude and temperature dependence. While the first two probe nodal quasiparticles at the (□, □) points of the k-dependent d-wave density of states at an energy scale of ~k_BT, most pump-probe experiments excite the HTS with 1.5 eV photons whose energy is ~200 k_BT_c and the cascade can include all k states. In addition, the probe response, which measures the reflectivity changes after optical pumping, varies dramatically with probe frequency (even changing sign) so the specific property of the nonequilibrium distribution being addressed is less clear. One expects that these probe-frequency dependencies will reflect features of the electronic system such as the plasma frequency as well as the changes due to these nonequilibrium states. For example, the temperature dependence of the amplitude of the 90 meV probe energy response to a 1.5 eV pump energy[133], shows a strong correlation with the amplitude of the neutron resonant spin excitation[139]. The resolutions of these fascinating mysteries promise a rich new field of research that can bring considerable insight into non-thermal processes in electronic oxides and possibly into the mechanism of HTS. For these experiments, it seems that much could be answered if another probe, like tunneling, could be done on such fast time scales (~10 psec) to complement the optical data.

The eventual recombination and energy transfer to phonons has been addressed in mm-wave absorption measurements that probe the reflectivity at a frequency of ~0.3 meV. The authors find relaxation times in the 10^{-6} sec range and intuit a more significant bottleneck than LTS due to the unique properties of the nodal quasiparticles. They also suggest an analogy to the T relaxation process[140] found for He. The long relaxation time means that the traditional nonequilibrium effects found in LTS, which have addressed the effects of excess quasiparticle densities and/or branch imbalances between electron-like and hole-like quasiparticles, should be observable in HTS. Such nonequilibrium effects in high-temperature superconductors (HTS) comprise a research area that is ready for exploitation.

Numerous effects of perturbations by tunnel-junction injection of quasiparticles (unpaired electrons), microwave or optical illumination, etc. are readily observed in low T_c superconductors (LTS) and these have been understood in terms of electron-phonon scattering[137, 138]. This is consistent with the electron-phonon coupling mechanism for these superconductors. Occasionally the effects of direct electron-electron (Coulomb) scattering must also be considered. In HTS the situation is potentially much more interesting for at least two reasons. The d-wave symmetry of the order parameter admits a momentum-dependence to the quasiparticle energy spectrum and there are additional spin and charge excitations that have been suggested as potential candidate bosons for the attractive interaction. The latter excitations are seen by neutron scattering and would be expected to interact with quasiparticles. By studying the relaxation processes in nonequilibrium it may be possible to address the importance of these excitations if their effects on the relaxation of nonequilibrium quasiparticle distributions can be identified.

Nonequilibrium states are here classified as those states for which the quasiparticle (or, e.g., phonon) distribution exhibits an energy profile different from thermal equilibrium. No matter how high the energy of the fundamental excitation process, in a fairly short time the excess energy of the perturbation relaxes, predominantly, into a state for s-wave superconductors in which it resonates between phonons of energy 2Δ and quasiparticles of energy $\sim\Delta$. This is due to the high density of quasiparticle states near Δ in the BCS density of states and it results in a bottleneck for the escape of the 2Δ recombination phonons into the thermal bath since they are resonantly reabsorbed by the high density of Cooper pairs. This increases the effective recombination time above the bare value (typically by one to two orders-of-magnitude).

The observations of many diverse nonequilibrium effects observed in low T_c superconductors (LTS) benefit from the long time constants for the ultimate recombination into Cooper pairs. This is due to the 2Δ-phonon bottleneck and the small energy scale of Δ in LTS also contributes to a long bare recombination time due to the small phase space available in the decay channel via phonons (density of phonon states $\sim\Delta^2$). Nonequilibrium studies in LTS have discovered new effects, like energy gap enhancement by microwave or tunnel-junction injection, branch or charge imbalance and new applications, like weak-link Josephson devices, superconducting three-terminal devices and particle detectors. See Ref. 9 for more complete reviews of these topics. The greater richness of the interactions in HTS, together with the nonconventional order parameter, large energy gap and the naturally layered structure can be anticipated to provide additional phenomena and applications. Examples include the coupling of ac Josephson oscillations to phonons or the possibility of terahertz oscillators enabled by the coupling of coherent Josephson vortex flow in BSCCO to Josephson plasmons to produce electromagnetic radiation. For instance, in the latter case, one can test predictions of the occurrence of dynamically stabilized vortex configurations and the interaction with Josephson vortices with Josephson plasmons. In addition, the large energy gap in HTS cuprates make them attractive candidates to extend the frequency range of tunnel-junction mixers beyond that of LTS junctions. Although energy gap enhancement, by microwave illumination[141, 142] or tunnel junction injection[143], is well established in LTS, the discovery of photoinduced superconductivity in underdoped cuprates is unique and unexpected---it produces substantial increases in T_c that are persistent[14].

The large Δ_o in HTS, compared to LTS, may be expected to lead to shorter bare recombination times, but under many circumstances nonequilibrium effects can still occur. For example, the longer effective relaxation time due to resonant 2Δ-phonon adsorption mentioned above is largely a geometrical escape factor that may be quite similar[134] to that found in LTS. This resonant adsorption is usually referred to as phonon trapping since the nonequilibrium perturbation energy must be converted into, and carried away by, phonons. Phonons can be expected to play that same role in HTS, since, e.g., spin and charge excitations cannot leave the electronic system. But also, an additional trapping mechanism may occur due to the nodes of the d-wave order parameter. This proposed effect is the momentum-space analogy of the real-space quasiparticle traps devised for LTS superconductive detectors[144]. In such detectors, Cooper pairs in a large volume of superconductor (with a relatively large gap, $\square_l$) interact strongly with incident irradiation to produce excess quasiparticles. The detector is arranged so that the quasiparticles have a high probability of diffusing into an attached superconductor with a smaller gap, $\square_S$, before the energy escapes the system via phonons. The smaller $\square_S$ results in a *longer bare recombination time* due to the smaller phase space of phonons of energy $\square=2\square_S$. In addition, the excess energy of quasiparticles, $\sim\square_l$, converts into a greater number of quasiparticles with $E\sim\square_S$.

In a proposed relaxation mechanism, quasiparticles produced in the high-□ regions away from the nodes at the (□, □) points would diffuse to traps in momentum space at the lower energy states near the nodes. Several mechanisms can be envisioned, e.g., direct scattering of quasiparticles by phonons or spin excitations and pair breaking into near-nodal quasiparticle states by nonequilibrium phonons or spin excitations. The interpretation of nonequilibrium data in these regimes could be connected to models for the mechanism of HTS (see Chapter VII). It will be interesting to explore the relation of the specific momenta of spin excitations with relaxation processes across the d-wave Fermi surface. The multiplying factor upon energy degradation implies that a single 1.5 eV photon could create up to 4000 quasiparticles trapped at the nodal points with an energy scale of ~4 K. As pointed out above, measurable recombination times in excess of 10^{-6} sec have been reported in HTS.

The ease of fabrication of thin-film superconductor-insulator-superconductor tunnel junctions was also a vital component of previous studies of LTS materials. Making junctions with two HTS electrodes has proved much more difficult and most tunneling studies have relied on point-contact or STM tunnel junctions. However significant progress has been made using MBE growth of multilayers of HTS with lattice-matched insulators as well as the internal junctions of BSCCO crystals offer another opportunity that is unique to the HTS cuprates. In the latter case, it seems necessary to intercalate molecules (e.g., iodine or mercury bromide) between the Bi-O bilayers to reduce the current for injection near the energy gap, 2□, and avoid a significant weakening of the superconducting state[145].

VII. Theory

1. Preamble

Since the discovery of high T_c superconducting materials, there have been many ideas put forth to explain their unusual and often perplexing physical properties. Here, rather than attempting to survey the field, we offer three individual perspectives.

2. Phenomenological Approach

a) Status.

The cuprates are highly correlated systems close to the Hubbard-Mott antiferromagnetic insulating state. In the underdoped regime, pseudogap signatures[28] go well beyond ordinary metallic behavior. Here we will limit the discussion to the optimally doped case where Hubbard-Mott modifications may not be so severe. In this case generalizations of techniques developed for ordinary superconductors may be applicable with appropriate modifications and give valuable insight. For conventional superconductors phonon structures in current-voltage characteristics of planar tunneling were exploited to derive a complete picture of the electron-phonon spectral density $\square^2F(\square)$ [146]. This function defines the kernels that enter the Eliashberg equations. The theory accurately predicts (at the 10% level) the many deviations from universal BCS laws which have been seen in a broad range of experiments[146]. Similar equations suitably generalized to include d-wave symmetry[23, 147, 148] can lead to an equally good understanding of the observed superconducting properties of optimally doped YBCO. In this approach the general framework of a boson exchange mechanism is retained with a boson exchange spectral density (denoted by $I^2\square(\square)$), to be determined from experimental data. In the high temperature oxides, rather than tunneling, including STM, the technique of choice has so far been the infrared conductivity, from which one can construct a model of $I^2\square(\square)$. [23, 147, 148] When applied to the conventional s-wave case the method reproduces the tunneling derived model for $\square^2F(\square)$[149, 150]. In the oxides the optical scattering is dominated by a fluctuation spectrum which is largely featureless and which extends over a large energy scale of order several hundred meV (the order of J in the t-J model). Such a spectrum is expected in spin fluctuation theories such as the nearly antiferromagnetic Fermi liquid (NAFL)[151, 152] or in the marginal Fermi liquid (MFL)[153].

In the superconducting state a new phenomenon has been identified. One finds increased scattering at some definite finite value of $\square$ associated with the growth of a new optical resonance in the charge carrier boson spectral density, the energy of which ($\square_n$) corresponds exactly to the energy of the spin resonance measured by inelastic neutron scattering (when available). This correspondence does not prove, but provides support for a spin fluctuation mechanism (rather than the MFL). Moreover the spectral density derived from the infrared data, (at T_c in optimally doped YBCO) shows a form characterized by a spin fluctuation energy $\square_{sf}$ [152]. This form is progressively modified by the growth of the resonance at $\square_n$ and attendant reduction of spectral weight at smaller energies as the temperature is lowered below T_c. The spectrum obtained depends on temperature (through feedback effects due to the onset of superconductivity)[154, 155], and leads to good agreement with observed properties of the superconducting state. While the generalized (for d-wave) Eliashberg equations are not as firmly grounded in the basic microscopic theory as in the phonon case, they do offer a phenomenology within which superconducting properties can be understood. These include the condensation energy per copper atom, the fraction of total spectral weight which condenses into Cooper pairs at T=0, the temperature dependence of the superfluid density, the peak observed in microwave data as a function of temperature and its shift in position with microwave frequency, the similar peak in the thermal conductivity, and the frequency dependence of the infrared conductivity

b) Key Issues and Opportunities.

An important issue for the future is to extend the calculations to the underdoped regime. There is as yet no systematic quantification of pseudogap effects and contradictory views exist as to their origin. In the preformed pair model[29] the pseudogap and superconducting gap have a common origin with the superconducting transition related to the onset of phase coherence. In the d-density wave model[156] (DDW) a new order parameter competes with superconductivity. Another problem that needs resolution is understanding the new ARPES data which have been interpreted as giving strong signatures of phonon effects[157-159]. The dressed quasiparticle energies must also contain important renormalization due to the spin fluctuations. Certainly a pure phonon model is incompatible with the infrared optical data. However, it is well known that transport and quasiparticle scattering rates are different. In transport, backward collisions assume additional importance in the depletion of current, as compared with quasiparticle scattering. The quasiparticle electron-boson spectral density may have important contributions from both phonons and spin fluctuations, while the transport spectral density may be dominated by spin fluctuations. An important aim for the future should be to achieve a common understanding of ARPES, optical and tunneling data simultaneously.

3. Numerical Studies of Hubbard and t-J Models

a) Status.

Numerical studies of the high T_c cuprate problem have been used to determine what types of correlations are significant in specific models. They have shown that the 2D Hubbard and t-J models exhibit antiferromagnetic[160, 161], striped domain wall[162], and $d_{x^2-y^2}$ pairing correlations[162-165]. The similarity of this behavior to the phenomena observed in the cuprate materials support the notion that the Hubbard and t-J models contain much of the essential physics of the cuprate problem.

This is really quite remarkable when one considers that these are basically two parameter models involving U/t or J/t and the doping x = 1-n. Furthermore, boundary conditions or added next-nearest-neighbor hopping terms can shift the nature of the dominant correlations showing that the antiferromagnetic, stripe, and pairing correlations are delicately balanced in these models, reminding us of the behavior of the materials themselves.

b) Key Issues and Opportunities.

While we have seen that many of the basic cuprate phenomena appear as properties of these models, the interplay of the various correlations and the nature of the underlying pairing mechanism remain open. Thus a key issue is to determine whether the underlying physics is to be understood in terms of spin-charge separation[166, 167], SO(5) symmetry[130], stripes[168], spin-fluctuation exchange[169], or whether additional phonon mediated interactions may play a supporting role[46, 170]. With the understanding which has been gained and with further development of computational techniques, we have the opportunity of addressing these issues. Here it is important to realize that the search for the appropriate theoretical framework for understanding the cuprates also includes seeking to determine what type of models (and ultimately materials) are described by various scenarios. For example, we would like to understand what types of strongly correlated models exhibit spin-charge separation or more generally some type of fractionalization. Is there a sufficient temperature range for strongly correlated 2-leg ladders to renormalize so that an SO(5) description is appropriate? Do stripes suppress or enhance pairing? What role do phonons play and how is the electron-phonon interaction affected by strong Coulomb interactions? What is the structure of the phase diagram for these models? What new materials or material modifications will the answers to these questions suggest?

It should also be noted that theoretical progress in first-principles band theory simulations of ARPES intensities in the high-T_c's has been made and the inclusion of the electron-phonon and strong correlation effects in these simulations can advance the interpretation of the data[171].

We are in a position to address these issues and we also have the opportunity to take advantage of more than a decade and a half of advances driven by the cuprate discovery. As part of this effort we need to continue the development of numerical techniques. We should also work to establish closer connections to the electronic structure and quantum chemistry communities for key information on the basic orbitals and effective parameters that enter model descriptions of real materials.

4. Electronic Structure

a) Status.

The discovery of superconductivity in MgB_2 and the subsequent response by the computational community demonstrated the remarkable progress that has been achieved in first principles calculations for the electronic properties of conventional (phonon mediated) superconductors. Indeed, $\alpha^2F(\omega)$ can now be calculated accurately for fairly complex materials using density functional methods. For example, first principles evaluation of the electron-phonon interaction was used to calculate the superconducting transition temperature of the simple hexagonal phase of Si under high pressure[172]. Not only can the electron-phonon coupling be obtained, but also complete phonon dispersion curves for the whole Brillouin Zone (BZ) are being calculated using perturbation theory (harmonic approximation). If anharmonic terms are important, frozen phonon calculations yield total energies as a function of the relevant lattice distortions. Indeed, structural phase transitions involving soft phonon modes are frequently analyzed via such total energy calculations. While phonon frequencies and eigenvectors are needed to

evaluate $\square^2$F($\square$), it is difficult to draw conclusions about superconductivity from phonon dispersion curves. It is interesting however, that first principles calculations of phonons in the cuprates have in general yielded good agreement with neutron scattering experiments (see for example [173]and references therein).

When Local Density Approximation (LDA) calculations were unable to produce the insulating antiferromagnetic state in the cuprate phase diagram[174], it became clear that new approaches for dealing with correlation and moving beyond standard band structure techniques were needed. The first of these new “band structure” approaches, the LDA+U method, introduces a Hubbard U term into the LDA equations, affecting the orbitals for which the correlations are strong[175]. The more recent LDA++, and Dynamical Mean Field Theory (DMFT) methods make a more direct attack at calculating the electron self-energy, $\square(\mathbf{k},\square)$ [176-179]. The computational resources for evaluating the dynamics are demanding, and while good progress is being made, results have only been obtained for prototype systems. Although there is not yet a satisfactory band structure based technique for treating spin fluctuations when going from the Mott-Hubbard insulating state to optimally doped high T_c materials, straight forward band structure calculations of the doped cuprates yield Fermi surface geometries in remarkably good agreement with precise angle resolved photoemission experiments. Band structure calculations have also been valuable in identifying the relevant orbitals and in estimating values of the parameters that enter more phenomenological models.

b) Key Issues and Opportunities.

A key ingredient in solving the Eliashberg equation for phonon mediated superconductivity is the simplification made possible by Migdal’s theorem. In exploring other boson mechanisms with higher frequency spectra the role of the retarded Coulomb interaction, $\square^{\square}$, needs to be revisited[180]. It has been suggested that for vanadium the effective $\square^{\square}$ is larger than expected because of the pair-breaking influence of spin fluctuations[181]. In the one band Hubbard model it has also been argued that strong correlations suppress the electron phonon coupling in $\square^2$F and transport quantities[182]. The recent angle resolved photoemission measurements which show mass renormalization for bands passing through the Fermi energy may provide a quantitative measure of the electron-phonon interaction for specific states[159]. A comparison with first principles calculated values would be most interesting.

There are many other questions, many identified in this document, which are now being approached with model Hamiltonians. While electronic structure practitioners are eager to participate in and learn from such studies, and to provide parameters and insights where possible, there is a strong desire to develop the apparatus required for a real first principles treatment of the phenomena. There are many insights and ideas that need to be developed first. Perhaps the situation today is not so different than in the early 1960s when the Fermi surface was considered exotic. The dividends from the investment in physics of that period are the basis for what is now considered "routine" materials science, with applications ranging from Stockpile Stewardship to material processing to drug design. Solving the "high T_c problem" will likewise result in valuable tools and insights leading to future applications.

VIII. Defects and Microstructure with an Eye to Applications

Crystal lattice defects and their organization on the scale of nanometers to micrometers ("microstructure" for short) play a very significant role in the science and technology of superconducting materials: [183-188] For one thing, defects are unavoidable in the world of "real materials," and it is vital to characterize their nature and distribution so as to understand their effects on superconductivity. It is also vital to control the defect distribution in the polycrystalline, large-scale microstructure of conductors since appropriate nanoscale defects are responsible for developing high critical current densities, J_c, within grains. But planar defects, especially grain boundaries, block grain-to-grain transmission of the current, dictating the geometry of conductors because of the sensitivity of J_c to strain defects, etc. Defects can also provide insights into fundamental questions, e.g., the use of grain-boundary junctions in the investigation of order-parameter symmetry in cuprate superconductors. HTS conductors are available from several companies worldwide and have been used to demonstrate large components of the electric power grid such as power cables, motors, transformers and fault current limiters. Josephson-junction devices and other electronic devices based on HTS technology are in an advancing state of commercial development. However, we are still far from understanding or being able to optimize HTS material properties in the way that we have learned to do for the workhorse conductor of LTS (Nb-Ti). The main point is that our ability to adequately control defects and microstructures is still rudimentary. Some of the remaining key issues derive from the anisotropic nature of the cuprates and their low carrier density. These characteristics result in inadequate magnetic flux pinning, percolative current flow past many interfacial barriers, inability to control the phase state, and a general lack of materials control.

Extensive investigation of the cuprates has developed a firm understanding of some of their microstructure-sensitive properties. First of all, it is painfully clear that crystallographic texture and phase purity must be tightly controlled for high J_c in cuprates. It also seems unavoidable that magnetic flux pinning at temperatures, above about 30K, is inadequate in the present conductor material, Bi-2223. It is just too anisotropic for magnetic field applications, though adequate for self-field use in power cables at 77K. YBCO has much greater potential for applications in fields at 77K than Bi-2223, because its mass anisotropy is about 7, rather than the ~100 of Bi-2223, even though it's T_c is 92 K rather than the 110 K of Bi-2223. By contrast it has been quickly established that MgB_2 has only a small anisotropy (values vary from about 2 to 7, though with a greater weight on lower numbers) and that grain boundaries are not serious obstacles to current flow. Flux pinning also appears to be strong, leading to high critical current densities in prototype wires. In many respects MgB_2 appears to be exactly what its 39 K T_c suggests, intermediate in properties between LTS and HTS, benefiting in particular from lower anisotropy and relatively insensitive to planar defects.

It is not surprising at all that understanding of defects in cuprate superconductors is such a hard-won commodity, because these are very complex materials (the most practically important material, Bi-2223 $(Bi,Pb)_2Sr_2Ca_2Cu_3O_{10-X}$) forms a 7-component system when embedded in Ag). The continued attention to grain boundaries and to the search to understand flux-pinning defects has enhanced and will continue to increase our knowledge of defects in complex oxides in a much wider context, e.g., the understanding of defects in manganites, ferroelectric perovskites, etc. Continued investment in the materials physics of defects in HTS materials is attractive, not just because of the implications for superconductivity technology

What, then, are some of the outstanding issues in this field and how can we solve them? We need a new phenomenology, which combines the new physics of HTS with a realistic description of defects and microstructure in these complex materials. At present, almost all of the phenomenological discussion of the effects of defects and microstructure on the superconducting properties of HTS materials is based on theoretical concepts appropriate to s wave LTS. How do defects in HTS materials really interact with correlated-electron phenomena, stripe-phases, and electronic phase separation? We will not understand the answers to such questions without a basic theory of defects in complex oxides that takes account of their complex electronic state and proximity to the metal insulator transition.

Knowledge of lattice defects and microstructure in HTS materials is mostly confined to YBCO (and other 123-structure cuprates) and to the 2212 and 2223 phases of BSCCO. Why stick to these “old favorites?” To a very large degree, this reflects a **“**tyranny of practicality and materials complexity,**”** which inhibits the development of a wider knowledge needed to understand broader aspects of the materials physics of HTS materials. Many HTS materials are much more complex to make and appropriate recipes for “good sample” manufacture are lacking. It is believed that much might be learned from infinite layer materials. For example, their structures are not neatly divisible into charge reservoir and superconducting blocks. Since grain boundaries in HTS are believed to be disruptive to current precisely because charge transfer to the conducting cuprate planes is perturbed, their study in infinite layers might be particularly valuable.

Many issues involving magnetic flux pinning in HTS materials remain to be clarified. Although much is known about the thermodynamics and phase-diagrams of vortex matter in HTS materials, (see Chapter IV), much remains to be learned about the elementary interactions between vortices and defects, e.g., the physics of the elementary pinning forces, f_p, for various types of defects and their systematic variation among various cuprates. Furthermore, the knowledge of the behavior of defects, such as dislocations and plastic flow in vortex lattices themselves, is mostly extrapolated from the LTS case and almost certainly needs revision in such strongly anisotropic cases as Bi-2223, where line vortices in LTS materials break up into largely, but not completely disconnected pancake vortices. Experiments need to be designed specifically to illuminate the fundamental nature of defect-vortex interactions in HTS materials. These would be particularly valuable when combined with parallel conductor development activities. The intermediate nature of MgB_2 makes the nature of elementary pinning forces, vortex-lattice elasticity and plasticity very interesting. Are these properties fundamentally different or similar to those of Nb_3Sn and other LTS intermetallic compounds? Does the complex electronic band structure and anisotropy of MgB_2 make it's flux-pinning fundamentally different from that in the A15 compounds?

What is learned about the interactions between defects and correlated-electron phenomena in HTS materials will pay dividends in a wider range of materials, e.g., manganites, and phenomena, e.g., magnetism and metal-insulator transitions. In fact, the interactions between defects and transport properties in the normal state of cuprates are very poorly understood, too. A better understanding here would greatly improve the ability to characterize the nature and concentration of defects in cuprates in a quantitative manner.

There are many needs and opportunities in the science of defects and microstructure of cuprates, in addition to the direct connection to superconductivity (e.g., flux-pinning and weak links). The latter provides the motivation for microstructural control, but understanding of the basic materials science of defects and microstructure is needed to exercise such control efficiently. Here, too, experiments and theory designed to gain basic understanding that can couple to the activity driven by practical considerations would be very valuable. For example, there is a considerable lack of serious theory and modeling, as well as of basic experimental studies, of the thermodynamics, kinetics, and mechanisms of nucleation and growth of epitaxial oxides of relevance to coated conductors (including buffer layers, etc.), despite there being a large amount of process development in this area. Understanding of the fundamentals of phase formation in cuprate systems is sparse. There is also a serious need for quantitative understanding of the elementary defects, such as point defects, dislocations, twin boundaries, stacking faults, etc., which are the "elementary particles" of microstructure in HTS phases. This, together with quantitative descriptions of microstructure and defect chemistry, is needed to develop an adequate phenomenology of current transport and flux pinning in HTS systems.

Another area of fundamental materials physics that is relatively unexplored for HTS materials is that of mechanical properties, especially elasticity, anelasticity, and fracture. There is a paucity of basic experimental data, and these complex materials require theoretical methods more advanced than those needed for simpler materials, including ferroelasticity, non-linear and microcontinuum elasticity, and models of non-linear lattice statics and dynamics. Furthermore, an understanding of the coupling of elastic strain fields to the superconductivity of HTS materials is needed to understand interactions between defects and superconductivity, as well as to predict the behavior of conductors in devices such as high field magnets where large stresses arise during device operation.

The quantitative description of HTS-based conductors also requires improved methods of modeling the physical properties of composites, including mechanical, thermal and electromagnetic properties. The latter is particularly challenging, involving current and magnetic induction distributions in polycrystalline, defect-containing, multiphase composites.

The discussion above indicates the great complexity of the defect physics and microstructural science of HTS superconductors, which are both of fundamental interest and of enormous relevance to practical applications. However, powerful instrumental tools are available to help meet this challenge, especially modern transmission electron microscopy and local scanning probe microscopies and spectroscopies. These tools now permit the characterization of atomic and electronic structure, as well as elastic strain fields, over length scales ranging from atomic resolution to micrometers. This affords an unprecedented ability to obtain images and spectroscopy of atomic, charge, and strain distributions, which will revolutionize our quantitative understanding of defects and microstructure. The use of such instrumental tools, together with microscale electromagnetic characterization, coupled with the development of HTS-appropriate theoretical phenomenology, has the potential to yield important new insights into this complex problem, with wider implications for many complex new materials of the future.

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