Instability and high-T_c superconductivity

by Mitsuo Kataoka

The interrelation between instability and a high superconducting transition temperature T_c is argued theoretically in order to construct a model for the origin of the high T_c in the perovskite-type oxides. It is shown that when two nearly degenerate bands overlapping on the Fermi energy ε_F become unstable against spontaneous splitting to give rise to a charge redistribution, effective interactions between two electrons in the same bands become attractive, and the attractive interactions are strongly enhanced by increasing the degree of instability. One cause of this instability is the electron–phonon coupling, which results in lattice-instability-enhanced superconductivity; another cause is the Coulomb interaction between electrons, which results in electron-instability-caused superconductivity. The latter mechanism is successfully applied to the perovskite-type high-T_c superconductors. Some guidelines for obtaining a high T_c are presented on the basis of the present idea.

Introduction

Many researchers in the field of superconductivity (SC) have been aware of the fact that relatively high values of the superconducting transition temperature T_c are often found in metallic compounds with some type of instability, such as the A15 compounds including V_3Si and Nb_3Sn. This type of high-T_c superconductor exhibits the martensitic transition, or highly unstable nature [1]. Similar interrelations between T_c and lattice instability can also be clearly observed in LaS_x-based [2] and VRu-based alloys [3], although their T_c's are lower than 10 K. In $BaPb_{1-x}Bi_xO_3$, SC appears only in mixed compounds, and the highest T_c (13 K) is attained near a critical concentration x_c at which the metal–nonmetal transition occurs [4]. Peculiar behaviors of electronic properties in CuCl, CdS, and NbSi have been attributed to unidentified SC with extremely high T_c [5]. The observed fact that those behaviors are strongly sample-dependent and irreproducible may also imply an interrelation between high T_c and instability. The prediction of a strong interrelation between T_c and instability was tested experimentally by Testardi in the Re–Mo system [6]: The thin film of $Re_{0.62}Mo_{0.38}$ which was prepared by use of a deposition method exhibited a high T_c ($\simeq$15 K) in a narrow region of the deposition temperature including a structural transition temperature. Testardi supposed that the preparation of samples at these deposition temperatures could leave the alloy system unstable. In the newly discovered perovskite-type compound systems with high-T_c SC [7, 8], many kinds of instability also occur, as is discussed in more detail in Section 2. These compound systems, therefore, are not exceptions to Matthias' statement that all high-T_c superconductors are "unstable" [9]. All of the experimental facts mentioned above allow us to consider a possibility of instability-enhanced (or -caused) SC.

Until now, many authors have tried to clarify theoretically the interrelation between SC and lattice or electronic instability. Cohen and Anderson [10] discussed the

maximum T_c on the basis of the formulas of T_c which are given by BCS theory [11] and by McMillan [12]. According to them, an increase of the electron–phonon coupling λ gives rise to a lattice instability, which prevents a compound from continuing to have a crystal structure favorable to high T_c: This limits the maximum λ or the maximum T_c instead of enhancing the T_c. However, not only the condition for the occurrence of an instability but also the expression of T_c has been altered by more advanced theories developed by Dolgov, Kirzhnitz, and Maksimov [13] and by Allen and Dynes [14]. The latter authors showed that T_c can increase with λ to exceed the limitation of T_c given by Cohen and Anderson, but that T_c is not enhanced by a phonon softening because it is governed by $(\lambda\langle\omega^2\rangle)^{1/2}$ (with an average of squared phonon frequency $\langle\omega^2\rangle$). See also [15]. Recently, Chakraverty [16] proposed another limitation of the maximum T_c which arises from the formation of bipolarons for large values of λ. These theories hold true for a general but simple system which consists of a single electron band and phonons. To look for T_c-enhancement mechanisms related to instability, we must consider each specific electron (or electron–phonon) system which exhibits an electronic instability or a lattice instability electronically driven.

This author proposed the SC enhanced or caused by instabilities [17–20]. In these SC mechanisms, it is assumed that nearly degenerate bands overlapping on the Fermi level split spontaneously through the electron–phonon coupling [the band Jahn–Teller (JT) effect] or through the Coulomb interaction. Several authors [21] have shown that SC can be caused or enhanced by multiband effects. In our mechanisms, however, the instability of systems plays an important role in causing high-T_c SC. The purpose of this paper is to discuss the applicability of our SC mechanisms to the perovskite-type oxide superconductors.

The paper is constructed as follows: In Section 2, we summarize many types of instability which have been found in $La_{2-x}M_xCuO_4$ and $YBa_2Cu_3O_x$. The mechanism for enhancement of SC by a lattice instability is explained in Section 3. We construct in Section 4 a model for the electronic structure of the perovskite-type high-T_c compounds in order to propose a high-T_c mechanism in which an electronic instability is important. Section 5 is devoted to concluding remarks, in which some guidelines for obtaining a high T_c are provided on the basis of the present high-T_c mechanisms.

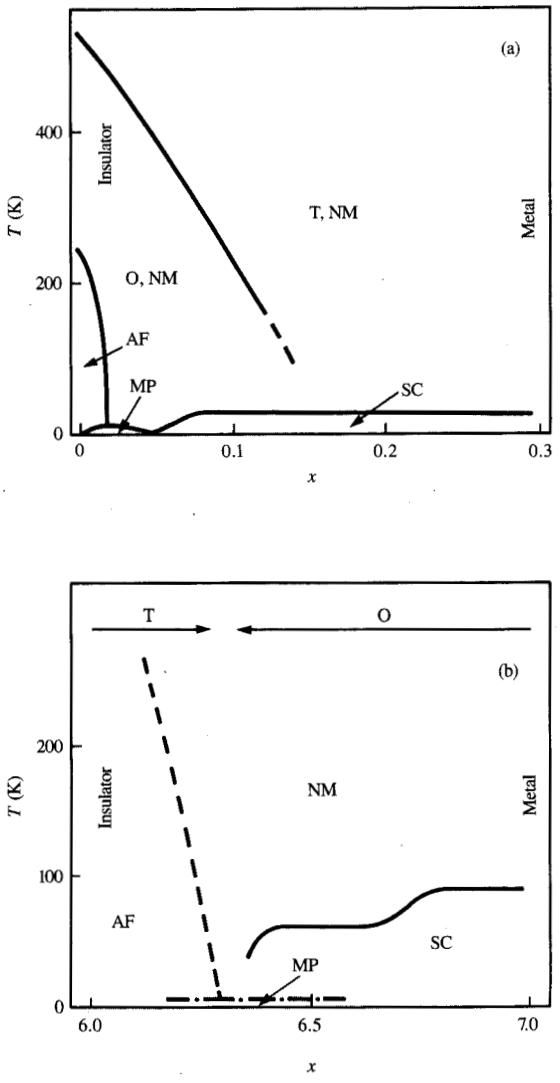

Figure 1

Phase diagrams of (a) $La_{2-x}Ba_xCuO_4$ [22] and (b) $YBa_2Cu_3O_x$ [23]. The abbreviations are as follows: AF, antiferromagnetic; MP, unidentified magnetic phase with no magnetic long-range order; NM, nonmagnetic; O, orthorhombic; T, tetragonal; and SC, superconducting.

2. Instabilities in the perovskite-type high-T_c oxides

Figure 1 shows the observed phase diagrams of $La_{2-x}Ba_xCuO_4$ [22] and $YBa_2Cu_3O_x$ [23]. As this figure shows, the two phase diagrams are very similar. This similarity, together with the fact that their crystal structures have common CuO_2 planes, strongly suggests a common high-T_c mechanism in both compound systems in spite of their very different T_c values. Because the phase diagrams are extraordinarily rich, three kinds of phase transitions (other than the superconducting phase transition) are found.

One of those transitions is the antiferromagnetic–nonmagnetic transition. The superconducting phase does not overlap the phase of the long-range antiferromagnetic order. However, local spins and spin fluctuations can also survive

in the superconducting phase. High-T_c mechanisms in which spin or exchange interaction is important were proposed by Anderson [24] and Emery [25].

The second transition is the tetragonal-to-orthorhombic (T–O) transition. The T–O transition accompanies the appearance of tiltings of oxygen octahedra in $La_{2-x}M_xCuO_4$ and the ordering of oxygens in $YBa_2Cu_3O_x$. Their transition temperatures $T_D \simeq 500$ K in La_2CuO_4 and $T_D \simeq 1000$ K in $YBa_2Cu_3O_x$ are much higher than the T_c's. When x is increased in the orthorhombic phase, T_D's are drastically decreased so that the lattice instability and SC can affect each other. In the case of $La_{2-x}M_xCuO_4$, the highest T_c appears near values of x at which T_D becomes comparable to T_c [22, 26]. On the basis of this fact, this author proposed a high-T_c mechanism in which the lattice instability enhances SC [18]. Although the applicability of this mechanism to $La_{2-x}M_xCuO_4$ is doubtful at present, we will describe this mechanism for an example of the lattice-instability-enhanced SC.

The third transition is the metal–nonmetal transition. In both compound systems, nonmetallic states at small values of x are changed by increasing x into metallic states which exhibit high-T_c SC. In the early stage of the study on these high-T_c superconductors, the transition into a nonmetallic phase was considered to be due to the formation of a charge-density wave (CDW) or a spin-density wave (SDW) through the Fermi-surface nesting in a half-filled two-dimensional band. Some authors [27] searched for enhancement mechanisms of SC by formations of CDW and SDW. Experiments performed until now, however, do not give any evidence of the existence of a CDW or SDW in these compounds. Therefore, the insulating behavior and also the existence of local magnetic moments are ascribed to strong Coulomb interactions between electrons. Nevertheless, high T_c's appear even in metals near the insulating phases. This fact implies a possibility that the strong Coulomb interaction itself or a charge redistribution caused by the Coulomb rather than electron–phonon interaction is responsible for the appearance of SC. By taking account of many experimental results on the electronic states in the high-T_c oxides, we construct a model for an electronic mechanism of the high-T_c SC in Section 4 [20].

3. Lattice instability and high-T_c superconductivity

Bednorz and Müller [7] expected that Cu^{2+} in the perovskite-type Ba–La–Cu–O system was a JT ion and that its strong electron–phonon coupling would raise T_c to a value higher than the T_c of $BaPb_{1-x}Bi_xO_3$. For the origin of the T–O transition observed in $La_{2-x}M_xCuO_4$, Barišić, Batisić, and Friedel, as well as Labbé and Bok [28], proposed a mechanism of the band JT effect to which two density-of-states (DOS) peaks originating from the van Hove singularities of the two-dimensional band pertain. This author showed that the lattice instability due to the band JT effect can enhance SC [18]. We describe the outline of this theory in the following, leaving its applicability to $La_{2-x}M_xCuO_4$ to the end of this section.

For a representative model of the band structure which exhibits a band JT effect, we assume two nearly degenerate bands which give two peaks of the DOS near the Fermi level ε_F but are split by both acoustic and optic phonon modes. (See **Figure 2**.) The band JT effect occurs when an energy gain by redistribution of electrons into the split bands overcomes an increase in the energy of ionic displacements. Therefore, it is required for occurrence of the band JT effect that the change in the DOS should be larger near ε_F so as to give a sufficiently large number of electrons participating in the JT effect [29].

The phonon-mediated interaction between electrons is assumed to be written as

$$H_{\text{int}} = \frac{1}{2V}\sum_{jj'}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}\sum_{\sigma\sigma'}\Gamma_{jj';jj'}(\mathbf{q},\omega)a^{j\dagger}_{\mathbf{k}+\mathbf{q}\sigma}a^{j'\dagger}_{\mathbf{k}'-\mathbf{q}\sigma'}a^{j'}_{\mathbf{k}'\sigma'}a^{j}_{\mathbf{k}\sigma}, \tag{1}$$

$$\Gamma_{jj';jj'}(\mathbf{q},\omega) = 2\sum_{s}\frac{\hbar\omega_{\mathbf{q}s}\alpha_{-\mathbf{q}s,j'j'}\alpha_{\mathbf{q}s,jj}}{(\hbar\omega)^2-(\hbar\omega_{\mathbf{q}s})^2}, \tag{2}$$

where V is the crystal volume, $a^j_{\mathbf{k}\sigma}$ is the annihilation operator of an electron with wave vector $\mathbf{k}$ and spin σ in the j (= 1 or 2) band, $\hbar\omega_{\mathbf{q}s}$ is the phonon energy while $\hbar\omega$ is the energy difference between incoming and outgoing electrons in the scattering process given by Equation (1), and $\alpha_{\mathbf{q}s,jj}$ is the coupling constant between a j electron and a phonon with wave vector $\mathbf{q}$ and polarization s. When the instability against a spontaneous ionic displacement accompanying the band splitting occurs at $\mathbf{q} = 0$,

$$\alpha_{\mathbf{q}s,11} \simeq -\alpha_{\mathbf{q}s,22} \tag{3}$$

and therefore

$$\Gamma_{11;11}(\mathbf{q},\omega) \simeq \Gamma_{22;22}(\mathbf{q},\omega) \simeq -\Gamma_{12;12}(\mathbf{q},\omega) \simeq -\Gamma_{21;21}(\mathbf{q},\omega) \tag{4}$$

holds at small values of $\mathbf{q}$ and $\omega < \omega_D$ (the Debye frequency). For simplicity, Equation (4) is assumed to hold even for larger values of $\mathbf{q}$.

The interaction constants $\Gamma_{jj';jj'}(\mathbf{q},\omega)$ are further renormalized to be $\overline{\Gamma}_{jj';jj'}(\mathbf{q},\omega)$ by exciting electron–hole pairs. After the renormalization is done self-consistently, we arrive at

$$\overline{\Gamma}_{jj';jj'}(\mathbf{q},\omega) = \frac{\Gamma_{jj';jj'}(\mathbf{q},\omega)}{S(\mathbf{q},\omega)}, \tag{5}$$

$$S(\mathbf{q},\omega) = 1 - \sum_{j}\Gamma_{jj;jj}(\mathbf{q},\omega)\Pi_{jj}(\mathbf{q},\omega), \tag{6}$$

$$\Pi_{jj}(\mathbf{q},\omega) = 2\sum_{\mathbf{k}}\frac{f(\varepsilon^j_{k+q})-f(\varepsilon^j_k)}{\hbar\omega+(\varepsilon^j_{\mathbf{k}+\mathbf{q}}-\varepsilon^j_{\mathbf{k}})}, \tag{7}$$

where $\varepsilon^j_{\mathbf{k}}$ is the energy of a j electron with $\mathbf{k}$, and $f(\varepsilon^j_{\mathbf{k}})$ is its Fermi distribution function. In obtaining Equation (5), we have used Equation (4).

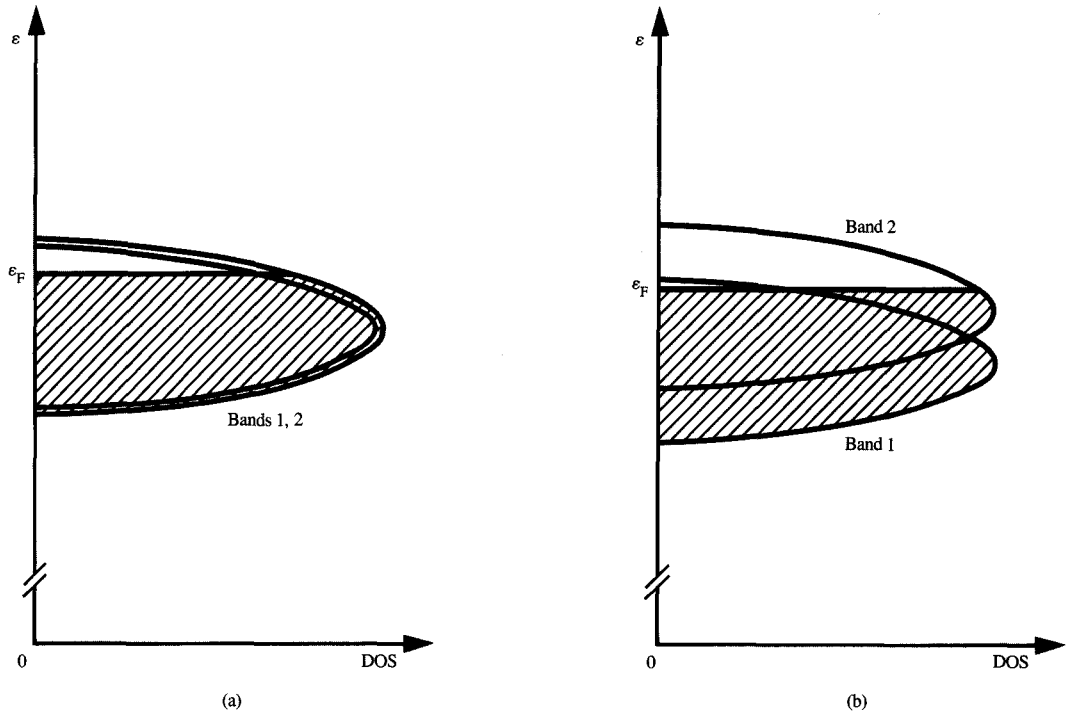

Figure 2

Schematic diagram of a band structure which exhibits the band Jahn–Teller effect. The nearly degenerate bands in (a) a crystal with no ionic displacement split to give rise to a charge redistribution in (b) a crystal with ionic displacements.

The phonon-mediated interaction constants $\Gamma_{jj';jj'}(\mathbf{q}, \omega)$ can have nonvanishing values at $\mathbf{q} = \omega = 0$ without violating the stability condition for the starting electron-lattice system. This is because the two forces that move the ions produced by the piling of electrons into the two bands up to the Fermi level cancel each other under the situation given by Equation (3). Nevertheless, the system becomes unstable if the harmonic potential of ions becomes sufficiently shallow because of the presence of the electron–phonon coupling and finally has a maximum, rather than minimum, value at the ionic positions in the starting crystal structure. Investigating the response of the electron system with the interactions $\Gamma_{jj';jj'}(\mathbf{q}, \omega)$ to a test charge, we find that the instability occurs when $S(0, 0)$ becomes zero. This instability can be realized in the two-band electron system with a strong electron–phonon coupling and/or high DOS at ε_F. The instability condition $S(0, 0) = 0$ and Equation (5) prove that the instability can strongly enhance the renormalized interactions between electrons at small values of $\mathbf{q}$ and ω. As shown in **Figure 3**, the renormalized interaction between two electrons in the different bands $\bar{\Gamma}_{12;12}(\mathbf{q}, \omega)$ becomes almost divergently repulsive, while that between two electrons in the same bands $\bar{\Gamma}_{jj;jj}(\mathbf{q}, \omega)$ becomes almost divergently attractive at small values of $S(\mathbf{q}, \omega)$ under the situation given by Equation (3). The divergent interactions at $\mathbf{q} = \omega = 0$ guarantee the spontaneous band splitting or electron redistribution accompanying ionic displacements. The strongly enhanced attractive interaction $\bar{\Gamma}_{jj;jj}(\mathbf{q}, \omega)$ with $\omega < \omega_D$ is here considered to cause a high T_c [30].

The excitation spectra of the electron-lattice system are determined from $S(\mathbf{q}, \omega) = 0$. Just at the "instability point," where the instability occurs, there exists a soft mode with its dispersion $\omega_{\mathbf{q}} \propto \mathbf{q}^2$, which consists of mixed motions of ions and electrons [29]. This mode corresponds to the so-called acoustic plasmon in a two-band electron system [30]. This soft mode, however, has a very short lifetime, since it is usually overdamped. Therefore, SC has been enhanced by the use of individual electron excitations rather than the acoustic plasmon. The presence of the Coulomb interaction between electrons does not affect the enhancement mechanism of SC discussed above. The reason for this is as follows: The instability is achieved, in general, through an

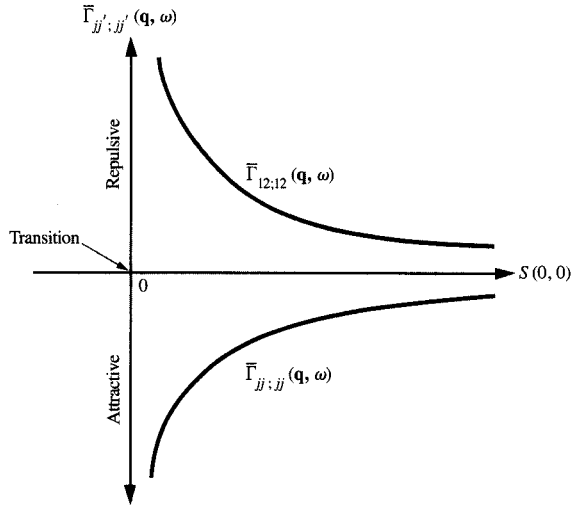

Figure 3

Renormalized phonon-mediated interactions $\bar{\Gamma}_{jj';jj'}(\mathbf{q}, \omega)$ between electrons in the two bands specified by $j = 1$ and 2. It has been assumed that the instability occurs at $\mathbf{q} \to 0$, and $\mathbf{q}$ and ω in this figure are sufficiently small. The considerable enhancement of the interactions originates from the instability caused by spontaneous band splitting.

effective electron–electron interaction including both phonon-mediated interactions and Coulomb interactions. So long as the instability accompanying a spontaneous band splitting does occur, the divergent attractive interaction should always result. As deduced from the above arguments, a larger enhancement of SC can be expected for a "soft" electron-lattice system, i.e., a system with a high degree of instability. Therefore, an instability near a continuous (or second-order-like) transition and a two-dimensional electron system are favorable for a higher T_c.

According to recent ultrasonic experiments [31], the high-T_c compounds exhibit some anomalies in the temperature dependences of sound velocities, but those anomalies are much weaker than those observed in some A15 compounds with the band JT effect. Neutron-diffraction experiments show that the phonon DOS [32] and the phonon dispersion [33] are only weakly temperature-dependent on the low-energy side. Very recently, Böni et al. [34] proved by use of neutron inelastic scattering experiments that the TO transition in $La_{2-x}Sr_xCuO_4$ is caused by a soft-phonon transition at the X point similar to that observed in many perovskites. Although the coupling between electrons and the soft mode has not yet been clarified, the origin of the transition may not be found in the system of electrons near the Fermi level. If this is true, the present enhancement mechanism of SC cannot be applied to $La_{2-x}M_xCuO_4$ even if the theory is extended to the case of the instability at $\mathbf{q} \neq 0$. It remains to investigate the applicability of this mechanism to some other compounds exhibiting electronically driven lattice instabilities [35]. This mechanism, however, together with the electronic mechanism of SC which is discussed in the next section, may lead to an understanding of the interrelation between instability and SC.

4. Electronic instability and high-T_c superconductivity

The band structure calculations [36] show that La_2CuO_4 has a half-filled band near ε_F and can be a metal. The real La_2CuO_4, however, is an insulator and has local magnetic moments on Cu sites [see Figure 1(a)]. Breaking down the results of the band structure calculation indicates that a strong electron correlation plays a decisive role in the electronic states of the high-T_c oxides. The following currently available experimental results give us information on the electronic states realized in the strongly correlated electron system. Shafer, Penney, and Olsen [37] used a chemical method to show that holes created by doping Sr^{2+} in La_2CuO_4 enter [Cu–O] complexes, resulting in $[Cu–O]^+$. Nücker et al. [38] observed O 1s absorption edges in $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{7-y}$. They found that the nonvanishing DOS's of oxygen hole states appear in both mixed compounds exhibiting SC. Most of the many results for XPS and XAS have shown the coexistence of $Cu^{2+}(d^9)$ and $Cu^{1+}(d^{10})$ but no existence of $Cu^{3+}(d^8)$ [39]. A positive Hall coefficient and a negative diffusion thermopower observed in highly doped $La_{2-x}Sr_xCuO_4$ imply the presence of both holes and electrons. The concentration of electrons increases with increasing Sr content [40].

On the other hand, it has been shown by many band calculations for the high-T_c compounds that the CuO_2 plane, which is a common frame in all structures of the high-T_c compounds, supplies electronic bands consisting of Cu 3d and O 2p orbitals on the Fermi level. Taking account of the result of the band calculation for La_2CuO_4 [36], it is assumed here that the orbital $d_{x^2-y^2}$ (pointing toward O sites in the CuO_2 plane) with the energy "ε_d" on Cu sites and the orbitals p_x and p_y (pointing toward Cu sites) with the energy "ε_p" on O sites are important for the electronic states near the Fermi level. We apply the tight-binding approximation to the CuO_2 plane to find one bonding, one antibonding, and one nonbonding band. The transfer integral between Cu and O is not sufficiently large compared with $|\varepsilon_p - \varepsilon_d|$, as seen from the result of the band calculation [41]. For $\varepsilon_p > \varepsilon_d$, therefore, the bonding and antibonding bands are dominated by the d and p characters, respectively. In order to reproduce the half-filled band near the Fermi level [36], one hole (per unit cell) is attached to the three tight-binding bands.

To accommodate the experimental facts stated above and the obtained tight-binding electronic structure, we assume

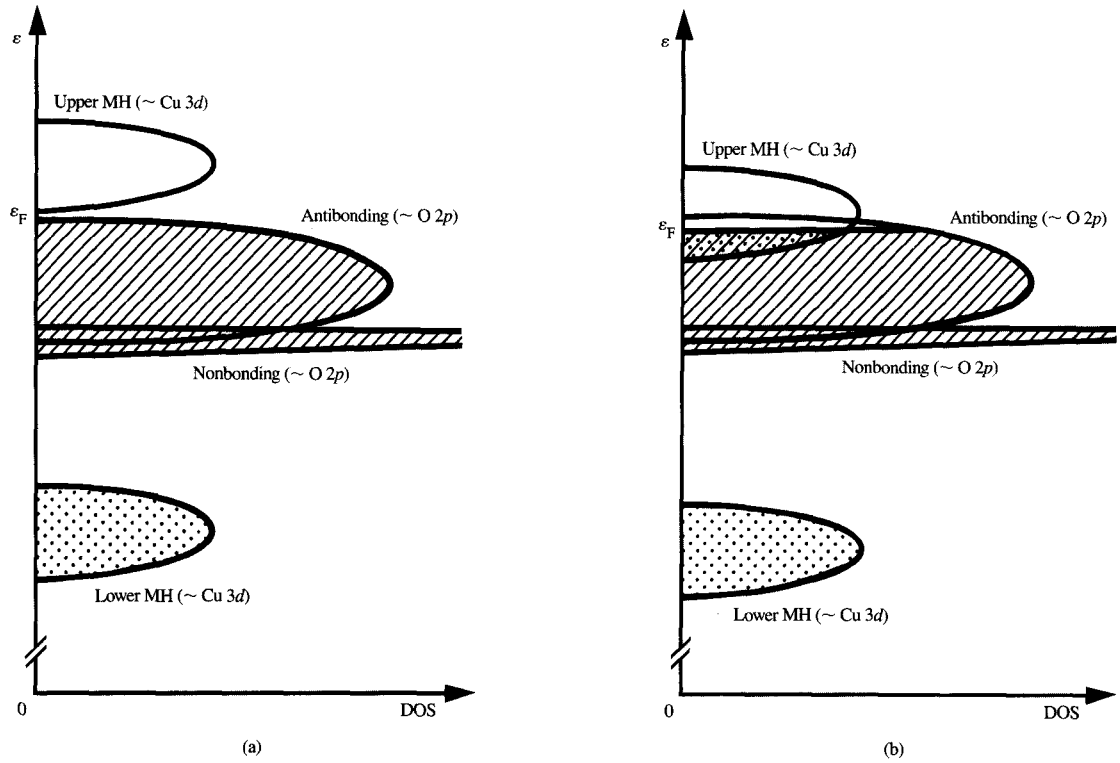

Figure 4

Model for the electronic structure of the perovskite-type oxide systems with high T_c's. The orbitals of Cu $3d$ and O $2p$ spreading in the CuO_2 plane have been taken into account. The bonding band of Cu $3d$ and O $2p$ has been assumed to be split into the upper and lower Mott–Hubbard (MH) bands by a strong Coulomb correlation on Cu sites. The empty upper MH band in (a) an insulating phase is shifted to overlap the antibonding band in (b) a metallic phase.

that the bonding band splits into lower and upper Mott–Hubbard (MH) bands [38] and that the upper MH band lies just above the antibonding band in the insulating state, as depicted in **Figure 4(a)**. In the metallic state realized by doping of holes, however, we assume that the upper MH band and the antibonding band are shifted to overlap each other as depicted in **Figure 4(b)**. This electronic structure scheme is consistent with the observed mixed-valence nature [39] and the existence of two types of carriers [40]. The most important character of the two electronic structures in Figures 4(a) and 4(b) is that a transition between them is possible by changing the hole concentration, as is shown below [20].

We concentrate our attention on the overlapping upper MH and antibonding bands crossing the Fermi level in Figure 4(b), since we are interested in the mechanism of SC. In this electron system, there are three kinds of Coulomb interactions: the interaction between two electrons in the antibonding band, $V_{aa;aa}(\mathbf{q})$; that between two electrons in the upper MH band, $V_{uu;uu}(\mathbf{q})$; and that between an electron in the antibonding band and an electron in the upper MH band, $V_{au;au}(\mathbf{q})$. Among them, $V_{au;au}(\mathbf{q})$ is expected to be large because a matrix element of the Coulomb interaction between the bonding and antibonding bands includes on-site Coulomb repulsions; furthermore, the overlapping of $d_{x^2-y^2}$ on Cu sites and p_x or p_y on O sites is large. On the other hand, $V_{uu;uu}(\mathbf{q})$ is expected to be small because the Coulomb repulsion on Cu sites has been used to create the MH gap, and the on-site Coulomb repulsion between electrons in the upper MH band is prohibited under the Pauli exclusion principle (in the framework of Wannier representations of the electronic states).

By proceeding with the same calculations as those made in [17–18] and in Section 3, $V_{jj';jj'}(\mathbf{q})$'s are renormalized self-consistently to be $\bar{V}_{jj';jj'}(\mathbf{q}, \omega)$. As the result, $\bar{V}_{aa;aa}(\mathbf{q}, \omega)$ is expressed by

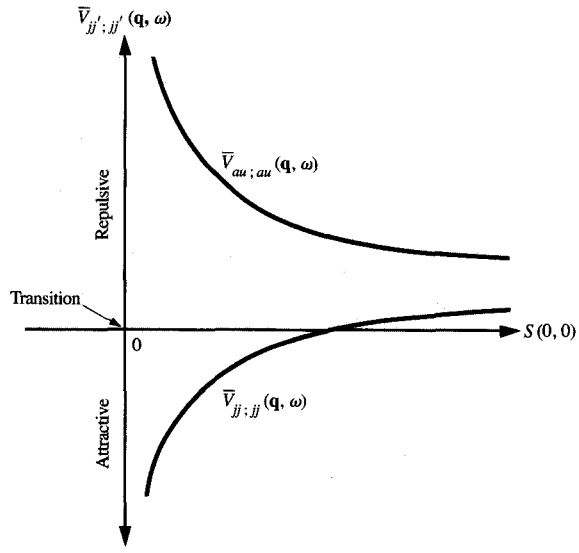

Figure 5

Renormalized Coulomb interactions $\bar{V}_{jj';jj'}(\mathbf{q}, \omega)$ between electrons in the upper Mott–Hubbard band $j = u$ and the antibonding band $j = a$. It is assumed that the instability occurs at $\mathbf{q} \to 0$, and q and ω in this figure are sufficiently small. The considerable increase in interactions originates from the instability caused by the spontaneous band splitting. It is noted that $\bar{V}_{jj;jj}(\mathbf{q}, \omega)$ becomes attractive only in a restricted region of $\mathbf{q}$ and ω.

$$\bar{V}_{aa;aa}(\mathbf{q}, \omega) = \frac{1}{|\Pi_{aa}(\mathbf{q}, \omega)|}\left\{1 - \frac{1 + V_{uu;uu}(\mathbf{q})|\Pi_{uu}(\mathbf{q}, \omega)|}{S(\mathbf{q}, \omega)}\right\}, \quad (8)$$

$$S(\mathbf{q}, \omega) = 1 - V_{aa;aa}(\mathbf{q})\Pi_{aa}(\mathbf{q}, \omega) - V_{uu;uu}(\mathbf{q})\Pi_{uu}(\mathbf{q}, \omega) - [V_{au;au}(\mathbf{q})^2 - V_{aa;aa}(\mathbf{q})V_{uu;uu}(\mathbf{q})]\Pi_{aa}(\mathbf{q}, \omega)\Pi_{uu}(\mathbf{q}, \omega), \quad (9)$$

where $\Pi_{aa}(\mathbf{q}, \omega)$ and $\Pi_{uu}(\mathbf{q}, \omega)$ are expressed like $\Pi_{jj}(\mathbf{q}, \omega)$ in Equation (7). $\bar{V}_{uu;uu}(\mathbf{q}, \omega)$ is obtained by the same method. However, we do not go into detail concerning $\bar{V}_{uu;uu}(\mathbf{q}, \omega)$, since the formation of the singlet Cooper pairing is difficult for a pair of electrons in the upper MH band.

The Fermi level is assumed to lie near the top of the antibonding band and the bottom of the upper MH band rather than at the centers of these bands. When the hole number is decreased by changing concentrations of dopants or constituent elements, $|\Pi_{aa}(\mathbf{q}, \omega)|$ decreases, but $|\Pi_{uu}(\mathbf{q}, \omega)|$ increases abruptly for small values of $\mathbf{q}$ and ω so that $|\Pi_{aa}(\mathbf{q}, \omega)\,\Pi_{uu}(\mathbf{q}, \omega)|$ can have large values for a region of hole concentration. On the other hand, the Coulomb interactions in the present characteristic electronic bands can realize

$$V_{au;au}(\mathbf{q})^2 - V_{aa;aa}(\mathbf{q})V_{uu;uu}(\mathbf{q}) > 0. \quad (10)$$

These and the smallness of $V_{uu;uu}(\mathbf{q})$ prove that $S(0, 0)$ obtained from Equation (9) can become zero at a finite number of holes [42]. At $S(0, 0) = 0$, a spontaneous band splitting or a cooperative flowing of electrons in the upper MH band into the antibonding band occurs, as proved by making the same arguments as in the preceding section. The transition occurs in order to avoid the strong interband Coulomb interaction $V_{au;au}(\mathbf{q})$ by prohibiting coexistence of the different kinds of electrons. It is noted that this band splitting results in a charge redistribution between Cu and O sites but does not give rise to any change in the crystal symmetry.

As seen from Equation (8) and **Figure 5**, $\bar{V}_{aa;aa}(\mathbf{q}, \omega)$ becomes attractive for

$$S(\mathbf{q}, \omega) < 1 + V_{uu;uu}(\mathbf{q})|\Pi_{uu}(\mathbf{q}, \omega)|, \quad (11)$$

although $\bar{V}_{au;au}(\mathbf{q}, \omega)$ remains repulsive. The divergent behaviors of $\bar{V}_{jj';jj'}(0, 0)$ at $S(0, 0) \to 0$ again guarantees the spontaneous band splitting. The attractive interaction $\bar{V}_{aa;aa}(\mathbf{q}, \omega)$ with small values of $\mathbf{q}$ and ω which is caused by the instability is considered to be responsible for the high-T_c SC in the perovskite-type oxides. The condition $S(\mathbf{q}, \omega) = 0$ under $S(0, 0) = 0$ again gives the dispersion of the soft acoustic plasmon as $\omega_{\mathbf{q}} \propto \mathbf{q}^2$. This mode, however, is overdamped, so that the attractive interaction is attained by use of individual electron excitations. Equation (11) means that only electrons whose energies lie in a limited region, say, between $\varepsilon_F - \varepsilon_D$ (>0) and $\varepsilon_F + \varepsilon_D$ can form Cooper pairings. The cutoff energy ε_D plays the same role as $\hbar\omega_D$ in the phonon mechanism. (See [20] for more details.) The attractive interaction obtained here has a purely electronic origin and is enhanced by instability, tending to produce a high T_c. A numerical estimation of T_c will be given by this author [20]. The electronic states in the high-T_c oxides are still highly controversial; in all high-T_c oxides, however, we expect at present that an instability leading to charge redistribution due to the Coulomb repulsion results in the high T_c, although the details of the electronic states near the Fermi level may be modified for each high-T_c compound.

5. Concluding remarks

In the preceding sections, we have shown that an instability due to a spontaneous splitting of overlapping bands on the Fermi level should result in attractive interaction between the same kinds of electrons, no matter the origin of the instability, and also that the attractive interaction is strongly enhanced by increasing the degree of instability. Such instability can be realized only for pairs of bands with strongly different characters. One example of these bands is the system consisting of two kinds of electrons which have strongly different effective masses. This electron system was assumed for A15 compounds with high T_c's [17]. In the electron system with the band JT effect, it is important that

the two bands have the electron–phonon couplings with different signs. In the electron system with the instability due to the presence of the Coulomb repulsions, on the other hand, it is important that at least one of the intraband Coulomb interactions is sufficiently weak compared to the interband Coulomb interaction. If the instability occurs without the aid of the electron–phonon coupling, the mechanism of SC is purely electronic. Since, however, the charge redistribution couples to phonons in general, phonons also contribute somewhat to the appearance of SC.

From the present mechanism, we deduce some guidelines for obtaining a high T_c:

1. Find metallic compounds with an electronic instability or a lattice instability which is electronically driven. It is possible to find SC with a high T_c in some of these compounds.
2. A second-order-like (i.e., continuous) transition as a function of concentrations, pressures, and so on is favorable.
3. Cause the compound system to approach the instability point to increase the degree of instability.
4. Do not stabilize the compound system, but sustain the unstable state.
5. A two-dimensional electron system is more favorable.
6. In the layered perovskite-type oxides, increase the density of the CuO_2 plane but do not lose the two-dimensional and unstable characters of the electron system.

Some of these guidelines for obtaining a high T_c are doubtless in accord with conclusions which have been reached by many experimentalists, confirming again the important role of instability in high T_c.

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42. $V_{jj';jj'}(\mathbf{q})$'s used here should be regarded as the unscreened Coulomb interactions, expressed by combinations of $\mathbf{q}^n$ with $n \geqq -2$. Since the term of $\mathbf{q}^{-4}$ cancels in $[V_{aa;aa}(\mathbf{q})^2 - V_{aa;aa}(\mathbf{q})V_{aa;aa}(\mathbf{q})]$, the most divergent terms in $[V_{aa;aa}(\mathbf{q})^2 - V_{aa;aa}(\mathbf{q})V_{aa;aa}(\mathbf{q})]$ and in $V_{jj;jj}(\mathbf{q})$ in Equation (9) are both proportional to $\mathbf{q}^{-2}$ at $\mathbf{q} \rightarrow 0$. (See [20].)

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Mitsuo Kataoka *Institute for Materials Research, Tohoku University, Sendai 980, Japan.* Dr. Kataoka received a Ph.D. from Osaka University in 1972. Since 1970, he has been a research physicist at the Research Institute for Iron, Steel, and Other Metals (now the Institute for Materials Research) at Tohoku University. Dr. Kataoka was a visiting scientist at the Max-Planck-Institut für Festkörperforschung from 1987 to 1988. His research interests include magnetism, superconductivity, structural transition of solids, and alloy phases.