Mutual influence of structural distortion and superconductivity in systems with degenerate bands

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Abstract

The interplay between the band Jahn-Teller distortion and the superconductivity is studied for the system whose Fermi level lies in two-fold degenerate band. Assuming that the lattice distortion is coupled to the orbital electron density and the superconductivity arises due to BCS pairing mechanism between the electrons, the phase diagram is obtained for different doping with respect to half-filled band situation. The coexistence phase of superconductivity and distortion occurs within limited range of doping and the distortion lowers the superconducting transition temperature $T_c$. In presence of strong electron-lattice interaction the lattice strain is found to be maximum at half-filling and superconductivity does not appear for low doping. The maximum value of $T_c$ obtainable for an optimum doping is limited by the structural transition temperature $T_s$. The growth of distortion is arrested with the onset of superconductivity and the distortion is found to disappear at lower temperature for some hole density. Such arresting of the growth of distortion
at $T_c$ produces discontinuous jump in thermal expansion coefficient. The variation of strain with temperature as well as with doping, thermal expansion coefficient, the $T_c$ vs $\delta$ behaviour are in qualitative agreement with recent experimental observations on interplay of distortion and superconductivity in cuprates.

I. INTRODUCTION

The role of structural instability on the superconductivity had been a crucial question since the discovery of high temperature superconductivity [1]. Apart from the intermetallic compounds [2], the structural transition associated with the lowering of crystallographic symmetry has also been observed in high-$T_c$ cuprates [3,4] and fullerenes [5]. The existence of orbital degeneracy with the Fermi level (FL) lying within a degenerate band is a common feature to all these systems. Now for almost any set of degenerate electronic states associated with a molecular configuration there will exist some symmetry breaking interaction in which molecular distortion is associated with the removal of electronic degeneracy – goes by the name of Jahn–Teller theorem. Associated with such transition there is a change in the electronic density of states (DOS) around the FL and therefore, it is expected that the band Jahn-Teller (BJT) distortion would strongly influence the superconductivity in such a system. If the FL lies at the centre of the degenerate band then the DOS at the FL will be reduced drastically and the superconducting (SC) transition temperature $T_c$ will be reduced. On the other hand, $T_c$ can also be higher as phonon softening due to the BJT effect may increase the coupling constant which is inversely proportional to mean square phonon energy.

The dependence of $T_c$ on structural properties is less understood. There is a large number of growing experimental evidence indicating the strong mutual influence of structural distortion and superconducting transition. In fact, Bednorz and Müller in their historic paper conjectured that a J-T type of polaron formation may lead to high-$T_c$. Indeed, ex-
periments indicate that in $(La_{1-x}M_x)_2CuO_4$ (M = Ca, Ba, Sr) with the onset of $T_c$ around 38K each $CuO_6$ octahedron is distorted with interlayer $Cu - O$ distance equal to 1.9$\rho_A$ and an elongated $Cu - O$ distance of 2.4$\rho_A$. A detailed neutron scattering measurement of the temperature dependence of the spontaneous strain has been reported by Mck Paul et al,\[4\] for $La_{1.85}Ba_{0.85}CuO_4$ ($T_c \approx 38K$). The system exhibits a structural transition at 180 K; the magnitude of the strain rises on lowering temperature and shows an anomalous suppression below 75K. Although the suppression of the lattice distortion appears at a temperature higher than $T_c$, it is expected that this anomaly is associated with the appearance of superconductivity. Such structural transition has also been observed in other high $T_c$ compounds and its strong influence being correlated with the superconductivity by many authors\[7]. The evidence for such interplay between lattice distortion and superconductivity in $La_{1.85}Sr_{0.85}CuO_4$, $YBa_2Cu_3O_6.5$ and even in the electron doped cuprate system $Nd_{1.85}Ce_{0.15}CuO_{4-\delta}$ has been reported by Lang et al,\[8\] from thermal expansion measurements. These measurements while demonstrating the insensitivity of structural distortion to charge carriers doping clearly exhibits that the highest $T_c$ is limited by lattice instability. Furthermore, the suppression of lattice distortion in the SC state has also been seen from extended absorption of X-ray fine structure edge measurements in the other families of cuprates e.g, the ‘2212’ and ‘2223’ Bi-superconductors\[9\].

The structural transition from tetragonal to orthorhombic phase in $La_{2-x}Sr_xCuO_4$ takes place at a temperature higher than the superconducting transition temperature. The transition leads to a change of bond distance in $CuO_2$ plane and the orthorhombic strain $\frac{a-b}{a+b}$ where $a$ and $b$ are bond lengths in the $CuO_2$ plane is the measure of distortion. Recently this distortion is measured in $La_{2-x}M_xCuO_4$ (M = Ca, Sr) as a function of doping ($x$). The structural transition is found to decrease with $x$ and also it causes suppression of $T_c$. The distortion decreases with $x$ in the superconducting phase and is completely suppressed at a critical value of $x$\[10\]. These measurements are clear demonstration of strong interplay between superconductivity and structural distortion\[10,11\].
In order to have a qualitative understanding of the interplay between the SC state and distortion, we present in this communication a detailed study of the coexistence of superconductivity and the BJT distortion for systems having FL lying in a two fold degenerate $e_g$-band, as a function of hole concentration. We find that, many unusual experimental findings like spontaneous suppression of strain close to $T_c$, kink like structures in the thermal expansion coefficient, $T_c \sim \delta$ behavior and the role of ionic size of the substituent ion on phase diagram etc. follows from this model. In the next section we present the model calculation for our results briefing the essential ingredients of our model and its inputs. Section 3 is devoted to analyze the calculated results so that a qualitative comparison can be made with the observed one. Finally, we conclude in section 4.

II. MODEL & CALCULATION

It is generally believed that in high temperature superconductors the electrons in $CuO_2$ layers contribute most to normal and superconducting properties. Experimental evidences also suggest that these charge carriers occupy mainly the $p$-state of oxygen. These electrons are also coupled to lattice as the site energy would depend on the state of the $CuO_2$ layer. In the tetragonal phase, electrons will ‘see’ the same site energy in ‘a’ and ‘b’ directions. However, orthorhombic distortion will remove such degeneracy of site energy as the ligand field would shift the energy level differently in a and b direction of a unit cell. Such distortion will alter the electronic states, energy and thereby will influence superconductivity. A realistic description of $CuO_2$ layer needs a five states model study to examine interplay between superconductivity and lattice distortion, becomes an involved one. Instead we study a simple and tractable model that incorporates essential effect (removal of orbital degeneracy) of distortion and superconductivity. We consider a model system where a two-fold degenerate ($e_g$) orbital is associated with each lattice point. The orbitals are strongly coupled to lattice and forms a band. This Jahn-Teller Hamiltonian can be described by,
\[ H = \sum_{k,\sigma,\alpha=1,2} (\varepsilon_k - \mu) C_{k\alpha\sigma}^\dagger C_{k\alpha\sigma} + \sum_{k,\sigma} Ge(\hat{n}_{k1\sigma} - \hat{n}_{k2\sigma}) + \frac{1}{2} ce^2 \]  

(1)

The first term represents band energy of electrons in two fold degenerate band with \( \mu \) being the chemical potential. The second term describes the electron - lattice ligand potential due to distortion \( e \) which is coupled to population density of orbitals \( (n_{k\alpha}) \). The expansion in direction ‘\( a \)’ lifts the one-electron level of orbital (say -1) whereas that of label (say -2) goes down due to compression along \( b \)-direction. In the limit of zero-volume change such shift of levels is equal to \( 2Ge \) where \( G \) is the electron lattice coupling constant \([13]\).

The last term refers to that static elastic energy due to strain with ‘\( c \)’ being the relevant elastic constant. Therefore, because of the electron-lattice ligand potential due to distortion the original degenerate bands with energy \( (\varepsilon_k - \mu) \) now shifts to different subbands \( \varepsilon_{k,\alpha} = \varepsilon_k - (-1)^\alpha Ge - \mu \). We assume that some pairing interaction exists only within the same orbital and that the strength of the pairing interaction is same for both the orbitals. Such pairing interaction may be written as,

\[ H_p = \sum_{k,k',\alpha,\alpha'} V_{k,k',\alpha,\alpha'} C_{k\alpha\sigma}^\dagger C_{-k\alpha\sigma}^\dagger C_{-k'\alpha'\sigma} C_{k'\alpha'\sigma}^\dagger \]  

(2)

with \( V_{k,k',\alpha,\alpha'} = -V\delta_{\alpha,\alpha'} \) and exists only within a cut-off energy \( \pm \omega_D \) around the Fermi level. So, within the mean field approximation, the model Hamiltonian and superconductivity may be obtained from equations (1) and (2) as,

\[ H = \sum_{k,\alpha\sigma} \varepsilon_{k\alpha} n_{k\alpha\sigma} + \sum_{k,\alpha}(\Delta C_{k\alpha\uparrow}^\dagger C_{-k\alpha\downarrow}^\dagger + \Delta^* C_{-k\alpha\downarrow} C_{k\alpha\uparrow}) + \frac{|\Delta|^2}{V} + \frac{1}{2} ce^2 \]  

(3)

The superconducting order parameter \( \Delta = -\sum_k V < C_{k\uparrow}^\dagger C_{-k\downarrow} > \) satisfies the equation,

\[ 1 = \sum_{k,\alpha} \frac{V}{2\omega_{k\alpha}} \tanh(\frac{\beta \omega_{k\alpha}}{2}) \]  

(4)

where \( \omega_{k\alpha} = \pm \sqrt{\varepsilon_{k,\alpha}^2 + \Delta^2} \) are the superconducting quasi particle energies in different subbands. The equilibrium value of strain \( e \) is one that minimizes the free energy and it is given by,
\[ e = -\frac{G}{c} \sum_{k,\alpha} (-1)^\alpha \frac{\varepsilon_{ka}}{2\omega_{ka}} \tanh\left(\frac{\beta\omega_{ka}}{2}\right) \]  

(5)

Finally, the chemical potential is determined from the equation for number (n) of charge carriers and hence the hole concentration as,

\[ \delta = \frac{1}{N} \sum_{k,\alpha} \frac{\varepsilon_{ka}}{2\omega_{ka}} \tanh\left(\frac{\beta\omega_{ka}}{2}\right) \]  

(6)

The equations (4-6) are coupled integral equations of order parameters \( \Delta, e \) and \( \delta \). In order to understand the nature of the coexistence phase, these three equations are solved self-consistently numerically. The temperature dependence of the chemical potential \( \mu(T) \) is important in determining the strain and the SC gap parameter self-consistently which has been taken care such that the calculated value of \( \delta \) differs from the given value of \( \delta \) at best at the fifth decimal point. This is carried out by replacing the \( k \)-summation by an integral over \( \epsilon \) with an appropriate density of states \( \rho(\epsilon) \). To simulate the strong energy dependence of \( \rho(\epsilon) \) around the centre of the band in the quasi two dimensional system we substitute \( \rho(\epsilon) = \rho(0)\sqrt{1 - \frac{\epsilon^2}{B^2}} \ln \left|\frac{B^2}{\epsilon^2}\right| \) with \( \rho(0) = (\int_{-B}^{B} \rho(\epsilon)d\epsilon)^{-1} \). Also the attractive potential \( V(\epsilon) \) (that appears in equation (2)) is simulated by, \( V(\epsilon) = V_0\left[1 - \frac{(\epsilon - \epsilon_F)^4}{\omega_D^4}\right]^{1/2} \), in which \( \epsilon_F \) denotes the Fermi energy and \( V_0 \) the strength of the pairing potential.

### III. RESULTS AND DISCUSSIONS

The coexistence of the BJT and the superconductivity is studied mainly by self-consistently solving the above set of coupled equations (4-6) for certain values of the input parameters \( G, \omega_D, c \) and \( B \) with varying hole concentration \( \delta \). The results presented below are derived with the dimensionless pairing potential \( \rho(0) V_0 = .11 \), the cut-off frequency \( \omega_D = 0.038 \) eV, the elastic stiffness constant \( c = 30 \) eV and the half-band width \( B = .1 \) eV. In this section, we first present the results that are obtained within our model and then discuss its close resemblance with the experimental observation later.

The thermal variation of the chemical potential at best small, is found to be important in determining phase diagram. Fig. 1 depicts the thermal variation of strain \( e \) for different hole
concentrations ($\delta$) (indicated in the figure) with a fixed value of electron-lattice coupling $G$ ($=1.16$ eV). It is seen that when the system is closed to half-filling (small $\delta$), the structural transition takes place at a quite high transition temperature ($T_s$). The strain grows with lowering in temperature and would have reached its maximum value at $T = 0$ if the system had remained in normal state (the curve with squares for non-superconducting (Non-SC) case). On the other hand, very different behaviour of $e$ is found when superconductivity occurs at lower temperature. The maximum value of strain is reached at the superconducting transition temperature $T_c$ for all doping and the maximum value decreases sharply with the increase in hole doping. The cusp-like behaviour of $e(T)$ at $T_c$ has important bearing in thermal expansion coefficient discussed later. For small $\delta$, $e$ saturates at low $T$ ($<< T_c$), and the saturation value at $T = 0$ decreases as dopant concentration goes up. Beyond a concentration which depends on model parameter strain disappears at lower temperature marking a re-entrant behaviour. This means that the system with higher value of $\delta$ goes from undistorted to distorted to undistorted phase transformation as temperature is lowered. The extent of suppression of strain depends sensitively on $\delta$ and the electron-lattice coupling strength $G$. The structural transition temperature $T_s$ goes down with $\delta$, and for $\delta = 0.3$ distortion does not appear.

The thermal variation of the superconducting order parameter $\Delta$ is presented in Fig. 2. To exemplify the effect of distortion on gap parameter the variation of $\Delta$ for $\delta = 0.1$ and $G = 0$ is also shown. The gap parameter is much reduced in presence of strain. It is also clear that $T_c$ is suppressed. For $\delta = 0.15$ the strain vanishes at lower $T$ ($< T_c$) leading to higher value of $\Delta$. The decrease in $\Delta$ at low $T$ ($<< T_c$) leading to higher dopant concentration is related to the decrease in the density of states at Fermi level in normal state. For reentrant situation a discontinuous growth of $\Delta$ is observed around a temperature where strain vanishes. It is also found that the BCS characteristic ratio is not constant and is higher than 3.5.

In Fig. 3(a) the hole concentration dependence of the strain at low $T$ ($<< T_c$) for
three different values of G is displayed. The magnitude of strain is highest for zero-doping system in which the Fermi level lies at maximum of the density of states. At first the strain decreases slowly for low $\delta$-regime. For $G = 1.16$ eV it vanishes shatply at a critical value of $\delta$ whereas in case of $G = 1.18$ & 1.2, it drops to zero discontinuously but at a higher value of $\delta$. The strain strongly depends on $G$ and increases monotonically with $G$ (Fig. 3b). Its value is nearly double for $\delta = 0.07$ when $G$ is increased by 4% only. Similarly, $T_c$ exhibits strong dependence on $G$ (Fig. 3 (c)) and decreases with $G$. The extent of decrease is larger for smaller value of $\delta$.

The dependence of superconducting transition temperature $T_c$ on hole concentration is presented in Fig. 4(a). In absence of BJT effect ($G = 0$ curve) $T_c$ decreases slowly with $\delta$. However, $T_c$ is much lowered in presence of distortion. The maximum suppression occurs at $\delta = 0$ and the extent of suppression is strong function of coupling strength $G$. It means that whereas the distorted-superconducting (D-S) phase exists for moderate value of $G$, the distorted-normal (D-N) phase can persist down to $T = 0$ with slightly higher value of $G$. Another important feature of this result is that the optimum doping concentration at which maximum $T_c$ is obtainable is different for different $G$. An interesting correlation between $T_c$ and strain at $T_c$ i.e $\epsilon(T_c)$ is observed and is depicted in Fig. 4(b). These quantities are obtained with different $\delta$ nearly collapse into a single curve over a range of $\epsilon(T_c)$. This correlation emphasizes the role of lattice distortion in determining $T_c$. Incidently, it is tempting to note that the such correlation namely lower $T_c$ in more distorted system has been observed in $La_{2-x}M_xCuO_4$ (M =Sr, Ca) compound [10].

The thermal expansion coefficient ($\alpha$) in this model system is much influenced by the interplay of strain and superconductivity. Apart from the normal contribution from the anharmonicity, the thermal variation of strain will contribute to $\alpha$. The thermal coefficient can be expressed as $\alpha = \alpha_{anh} + \frac{\partial \epsilon}{\partial T}$ where $\alpha_{anh} \approx \frac{\gamma C_v}{3 B}$ [12] ; $\gamma$ is the Grüneison parameter, $C_v$, the specific heat due to phonon and $B$, the bulk modulus. The first derivative of $\epsilon$ as obtained from the Fig. 1 for $\delta = 0.07$ and is shown in Fig. 5. At low temperature
$(T \ll T_c)$ $e$ is suppressed and is nearly independent of temperature (cf. Fig. 1) so $\frac{de}{dT}$ is nearly equal to zero. Therefore, at $T_c$, $\frac{de}{dT}$ has a discontinuity and the magnitude of discontinuity depends on $\delta$. Above $T_c$ it is negative and very large near $T_s$ and becomes zero again above $T_s$. This will produce a positive discontinuity at $T_c$ and a minimum at $T_s$ in the thermal variation of $\alpha$. The minimum is expected to be broadened in presence of fluctuation of strain parameter. This result is in qualitative agreement with experimental observation in oxide superconductors [8].

Finally, the phase diagram ($T_s, T_c$ vs $\delta$) is drawn in Fig. 6 for two close values of $G$. It shows the evolution of the distorted-normal (D-N), coexistence of distorted superconducting (D-S), undistorted superconducting (UD-S) phases as well as the re-entrance of the undistorted phase with hole concentration. In Fig. 6, the bold dots (solid line) represent the structural (superconducting) line indicating the respective phase boundaries. The transition temperature $T_s$, where distortion appears is highest for zero-hole concentration $\delta = 0$ (half-filled case). On the other hand, the superconducting transition temperature $T_c$ which is less than $T_s$ attains its maximum value at certain concentration. Below that concentration $T_c$ is much suppressed compared to its maximum value and is also suppressed compared to its value for undistorted phase. With the increase of $\delta$, $T_s$ decreases whereas $T_c$ goes up. The two transition temperatures become equal at a critical concentration of $\delta_c$ which depends on the values of the input parameters. Above $\delta_c$, the structural transition is completely inhibited by the onset of superconductivity and $T_c$ decreases again. Therefore, the highest value of $T_c$ is determined by structural transition temperature $T_s$ in accordance with the experimental observation [8]. Below $\delta_c$ a small region in $\delta$ characterized by vanishing of $e$ at low temperature is found. At $T = 20K$, the distorted phase appears at a concentration $\delta \leq 0.15$ which is less than $\delta_c$. Therefore, within this region of hole doping the phase transition from D-N to D-S to UD-S is observed with lowering of temperature. The re-entrant region shrinks with increasing value of $G$. In summary, the salient features of the phase diagram as follows from the model are:
(i) The spontaneous distortion appearing first at higher temperature interferes destructively with superconducting tendency of the system. However, the superconductivity co-exists with distortion within a certain region of parameter space.

(ii) With slight increase in electron-lattice interaction strength \((G)\) the superconductivity may be inhibited in a system with low doping (cf. Fig. 4(a) also)

(iii) a reentrant structural transition where system passes from undistorted normal phase to undistorted superconducting one through intervening distorted normal and distorted superconducting phases exist within small range of \(\delta\) (cf. Fig. 1 also).

(iv) The maximum value of \(T_c\) is limited by \(T_s\) and \(\delta_c\)

(v) The distorted phase does not appear if superconductivity occurs first.

The structural transition in this model results from the competition between lowering of the electronic energy due to lifting of the orbital degeneracy (band Jahn-Teller effect) and the increase in elastic energy associated with the strain. The lowering of electronic energy is associated with the redistribution of electronic states due to removal of orbital degeneracy. The net gain in energy on this process depends on the location of the Fermi level in the undistorted phase. When the lowering of the electronic energy due to distortion overwhelms the increase in strain energy, the spontaneous distortion appears in the system. The measure of this gain in energy is the structural transition \(T_s\) and this gain becomes largest when the Fermi level in undistorted phase lies at the maximum of the density of states. Both the transition temperature \(T_s\) and the strain \(e\) \((T = 0)\) are maximum for \(\delta = 0\) as the Fermi level lies at singular point of density of states. With the increase in hole concentration the Fermi level moves away from point of large density of states and this leads to lowering in \(T_s\) and \(e\). The suppression of the superconducting transition temperature in presence of structural distortion is related to removal of states from the Fermi level due to lifting of degeneracy. Larger the splitting of orbital states (higher values of \(T_s\) and \(e\)) larger is suppressive effect on \(T_c\). We note that the superconductivity can appear in system with or without distortion depending on electron-lattice coupling. However, it is clear that the
highest value of $T_c$ can be achieved in undistorted phase. With increase of hole concentration the suppressive effect (removal of states at the Fermi level) is diminished with consequent increase in $T_c$. In distorted-superconducting phase there is destructive interference between superconducting order parameter $\Delta$ and strain $e$. The lowering of strain in superconducting phase has to do with the appearance of energy gap across the Fermi level. The existence of the gap reverses the trend of lowering of energy due to structural distortion. The distortion is completely suppressed when the superconducting gap is larger than the orbital splitting energy $(2Ge)$. The reentrant behaviour at low temperature is the result of mutual influences between two order parameters. It is observed that the nature of the density of states and the location of the Fermi level are important ingredients in determining competing aspects of the superconductivity and the BJT like distortion. The maximum competing effect between the two order parameters can occur in the system with Fermi level located at energy where the density of states is large and sharply varying.

We would like to note that many salient features of the results are in tune with the trend of the experimental observations. The interplay between superconductivity and distortion has been distinctly observed in $La_{2-x}M_xCuO_4$ (M =Sr, Ca, Nd) [10]. The distortion at very low temperature decreases with increase in $x$ (hole concentration) and vanishes at a critical value of $x$. The $Ca-$substituted system is slightly more distorted than that for $Sr$-substituted one and at the critical value of $x$, the distortion vanishes with slight discontinuity in former compound in contrast to smooth vanishing for later one. For a fixed $Ca$ concentration, the distortion increases with $Nd$ concentration which replaces $La$. These results are similar in nature to those in Fig. 3(a,b) & 3(c), if it is assumed that the $Ca$-substituted compound has higher value of the electron-lattice coupling constant than that of $Sr$-substituted system. Similarly assuming $Nd$-substitution augments the value of G, the results of Fig. 3(a,b) simulates the observation that strain ($T_s$) increases (decreases with $Nd$ concentration). The higher value of G in $Ca$ ($Nd$) - substituted compound is related to lower value of ionic size of $Ca$ ($Nd$) which leads to smaller $La(Ca)-O$ ($La(-Nd)-O$) bonds. The smaller bond length
in turn increases the ligand field seen by hole. As G is determined by the rate of change of ligand potential one expects larger value of G for Ca(Nd) - compound in comparison to Sr-based compound. This assumption is consistent with experimental observation that the lower $T_c$ is found in more distorted Ca-system and $T_c$ decreases with Nd-substitution for doped (La – Nd) system [10]. The result that the increase in distortion lowers $T_c$ as observed in these systems [10,17] is in harmony with depicted in Fig. 3. Moreover, general features of the phase diagram (Fig. 5) are close to observed phase diagram in these system [10]. The fact that the highest $T_c$ is limited by $T_s$, the coexistence of superconductivity and distortion and complete suppression of superconductivity in system with large distortion are borne out from the model. For $G = 116$, $T_s$ varies little with $\delta$ and the maximum $T_c$ is $T_s$ at $\delta_c$. This correlates well with the observation in cuprates [8]. As noted earlier [10] the crucial quantity in the interplay between the two order parameters is the density of states at FL. The distortion produces a notch at FL which in turn lowers $T_c$. The notch gets deeper for larger distortion and so the larger suppression of $T_c$ results. As the FL shifts from singular point with doping the redistribution of DOS around FL is less marked and hence the suppressive effect of distortion on $T_c$ is lessened.

IV. CONCLUSION

In conclusion, a simple model based on orbitally degenerate band with electron-lattice coupling and the BCS-type pairing demonstrates the interplay between structural transition and superconductivity. It is found that the order parameters interferes destructively. The suppression of $T_c$ in the distorted phase is due to small number of states available at the Fermi level for pairing. The states at the Fermi level is depleted due to lifting of orbital degeneracy. This effect is highest when the Fermi level lies at the peak of the density of states. However, the distortion and the superconductivity can coexist in system for limited range of parameters of the model. The higher value of $T_c$ is found in system with lower value of distortion. With increase of hole concentrate $T_c$ increases and the distortion is completely
removed at a critical hole concentration. The value of $T_c$ at this concentration where $T_s = T_c$ is its highest value. The existence of the superconducting state at lower temperatures depend very sensitively on the strength of electron-lattice coupling. The effect of ionic size of iso-electronic $M$ (Sr, Ca, Nd) ion on the interplay of superconductivity and structural transition can be understood as the consequence of higher electron-lattice coupling. The electronic correlation effect are not discussed here and will reported elsewhere [16].
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