Short Communication

Elastic Properties of La$_{2-x}$Sr$_x$CuO$_4$ (x=0.10-0.20)

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Abstract

The expressions for elastic constant for high temperature superconductors, derived using Mie-Grüneisen interaction potential, are used to analyze the elastic properties (bulk modulus, elastic wave velocity) of La$_{2-x}$Sr$_x$CuO$_4$ for x = 0.10 to 0.20. The Debye temperature θ_D has also been computed which is found to decrease with increasing Sr concentration. The value of bulk modulus in superconducting phase (K_s) is larger than the value in its normal phase (K_n=113.8 GPa) for x = 0.10 to 0.14. After this limit K_s decreases. A simple empirical relation between the difference in bulk moduli in the two phases (superconducting and normal) and T_c is proposed. The value of T_c for La$_{1.85}$Sr$_{0.15}$CuO$_4$ obtained from the proposed relationship is in good agreement with the experimental value.

Keywords: Phase transition temperature; Debye temperature; High-temperature superconductor.

1. Introduction

The elastic anisotropy of K$_2$NiF$_4$ (2-1-4) type high temperature superconductors (HTSC) is a subject of much interest [1]. The general interest in high-T$_c$ superconductors has stimulated numerous experimental as well as theoretical investigations [2].The elastic constants of oxide superconductors [3] provide interesting information on long wavelength acoustic phonons, which enter in the basic superconducting mechanism. Because of this, there have been a number of studies [4-26] on these materials with the prospect of providing some insight into the mechanism of La$_{2-x}$Sr$_x$CuO$_4$. Fanggao *et al.* [27] stated that intermediate valence of Sr ions plays an important role in elastic properties

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of $La_{2-x}Sr_xCuO_4$ even though LSCO does not possess the highest known critical temperature.

The objective of the present investigation is to study the elastic properties (bulk moduli, Debye temperature) of $La_{2-x}Sr_xCuO_4$ for different Sr doping (x=0.10 to 0.20). With the help of computed values of bulk moduli, a simple relation between difference in bulk moduli in two phases (superconducting and normal) and T_c has been proposed. The computed values of T_c and Debye temperature are useful to analyse the electron phonon coupling constant λ.

2. Theory

The elastic properties are expressed by means of the derivatives of potential energy with respect to atomic displacements when the lattice is deformed. The development involves both translational symmetry of the lattice and the conditions of atomic equilibrium. The first order equations give the relative displacement of the various atoms in the unit cell, which occur when the crystal is strained uniformly. Expressions for the elastic constants can be obtained in terms of parameters of the generalized theory [28] by comparing the second order equations with the elastic equation for energy density using continuum approximation.

Elastic constants of all orders can be obtained as algebraic functions of potential parameters. Consider a crystal of large but finite volume V. The crystal is assumed to be free of any forces or stresses in the initial state. The potential energy of the crystal is expanded in powers of atomic displacements using Taylor series. Considering a two-body interaction during the homogeneous deformation of the lattice, the components of inter-atomic vectors are altered. The expression for the potential energy in terms of deformation parameters and component of the internal displacement of the sublattice is expressed as [24-26]:

$$
\begin{aligned}
\Delta\phi = \frac{1}{V_Z} 4K_2 \Bigg[& \sum_{L\mu}\sum_{L'\mu'}\sum_{ijkl} R_i\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_j\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_K\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_l\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} \eta_{ij}\eta_{kl} \\
& + \sum_{ij} \overline{W}_i(\mu)\overline{W}_j(\mu) R_i\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_j\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} \\
& + 2\sum_{ijk} R_i\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_j\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_k\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} \overline{W}_k(\mu)\eta_{ij} \\
& + \sum_{ijk} R_i\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} R_j\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} \overline{W}_k^2(\mu)\eta_{ij} \\
& + \sum_{ik} R_i\begin{pmatrix} L & L' \\ \mu & \mu' \end{pmatrix} \overline{W}_i(\mu)\overline{W}_k^2(\mu)\eta_{ij} \Bigg]
\end{aligned}
\tag{1}
$$

where V_Z is the volume of the unit cell. Eq. (1) becomes

$$\Delta\phi = K_2 \left\{ \sum_N \left[4\sum_{ijkl} R_i(N)R_j(N)R_k(N)R_l(N)\eta_{ij}\eta_{kl} + 4\sum_{ij} R_i(N)R_j(N)\overline{W}_i(N)\overline{W}_j(N) \right. \right.$$

$$\left. \left. + 8\sum_{ij} R_i(N)R_j(N)R_k(N)\overline{W}_k(N)\eta_{ij} + 4\sum_{ijk} R_i(N)R_j(N)\overline{W}_i(N)\overline{W}_j(N)\eta_{ij} \right] \right] \tag{2}$$

where N refers to the number of atoms in the unit cell. Substituting for the interatomic vectors of the nine nearest neighbours of each atom in the unit cell of $La_{2-x}Sr_xCuO_4$ in the matrices M_{ij} and D_{lkj}, we obtain the non-vanishing internal strain components:

$$\overline{W}_x(2) = \frac{7}{78}c\,\eta_{xz} \,, \; \overline{W}_y(2) = -\frac{5}{78}c\,\eta_{yz} \,, \; \overline{W}_z(2) = -\frac{3}{7}\frac{a^2}{c}\eta_{xx} - \frac{15}{49}\frac{b^2}{c}\eta_{yy} + \frac{675}{7938}c\,\eta_{zz}$$

$$\overline{W}_x(3) = \frac{11}{84}c\,\eta_{xz} \,, \; \overline{W}_y(3) = \frac{11}{84}c\,\eta_{yz} \,, \; \overline{W}_z(3) = \frac{33}{46}\frac{a^2}{c}\eta_{xx} + \frac{33}{46}\frac{b^2}{c}\eta_{yy} + \frac{36}{621}c\,\eta_{zz}$$

$$\overline{W}_x(4) = \frac{1}{12}c\,\eta_{xz} \,, \; \overline{W}_y(4) = \frac{1}{12}c\,\eta_{yz} \,, \; \overline{W}_z(4) = \frac{21}{46}\frac{a^2}{c}\eta_{xx} + \frac{21}{46}\frac{b^2}{c}\eta_{yy} + \frac{10}{69}c\,\eta_{zz}$$

$$\overline{W}_x(7) = -\frac{5}{78}c\,\eta_{xz} \,, \; \overline{W}_y(7) = -\frac{5}{78}c\,\eta_{yz} \,, \; \overline{W}_z(7) = -\frac{15}{49}\frac{a^2}{c}\eta_{xx} - \frac{15}{49}\frac{b^2}{c}\eta_{yy} + \frac{25}{294}c\,\eta_{zz}$$

$$\overline{W}_x(8) = \frac{5}{78}c\,\eta_{xz} \,, \; \overline{W}_y(8) = \frac{5}{78}c\,\eta_{yz} \,, \; \overline{W}_z(8) = \frac{3}{7}\frac{a^2}{c}\eta_{xx} + \frac{15}{49}\frac{b^2}{c}\eta_{yy} - \frac{25}{294}c\,\eta_{zz}$$

$$\overline{W}_x(13) = \frac{1}{12}c\,\eta_{xz} \,, \; \overline{W}_y(13) = \frac{1}{12}c\,\eta_{yz} \,, \; \overline{W}_z(13) = \frac{21}{46}\frac{a^2}{c}\eta_{xx} + \frac{21}{46}\frac{b^2}{c}\eta_{yy} - \frac{4}{69}c\,\eta_{zz}$$

$$\overline{W}_x(14) = -\frac{1}{12}c\,\eta_{xz} \,, \; \overline{W}_y(14) = -\frac{1}{12}c\,\eta_{yz} \,, \; \overline{W}_z(14) = -\frac{21}{46}\frac{a^2}{c}\eta_{xx} - \frac{21}{46}\frac{b^2}{c}\eta_{yy} - \frac{8}{69}c\,\eta_{zz}$$

The strain energy per unit volume in the undeformed state is obtained by substituting $\overline{W}_x$, $\overline{W}_y$ and $\overline{W}_z$ in Eq. (2) and dividing it by the volume of the unit cell V_Z.

$$U = \frac{1}{2!}\sum_{ijkl} C_{ijkl}\,\eta_{ij}\eta_{kl} + \frac{1}{3!}\sum_{ijklmn} C_{ij,kl,mn}\,\eta_{ij}\eta_{kl}\eta_{mn} \tag{3}$$

On comparing Eq. (2) and Eq. (3) and considering the atomic position, we get the required expressions for second-order elastic constants as

$$C_{11} = 474.45\,A; \quad C_{12} = 166.15\,A; \quad C_{13} = 108.80\,A$$
$$C_{33} = 291.00\,A; \quad C_{44} = 106.80\,A; \quad C_{66} = 159.00\,A \tag{4}$$

where $A = 48\ a^4 K_2/V_z$, K_2 is the second order force constants and V_Z is the volume and other symbols have their usual meanings [24-26].

2.1. *The Debye temperature*

The Debye temperature (θ_D) is closely related to many physical properties of solids such as specific heat and melting temperature. One of the standard method to calculate the Debye temperature is from elastic constants data, since θ_D may be estimated from the average sound velocity (v_m), by the following equation

$$\theta_D = \frac{h}{k} \left[\frac{3\,n}{4\,\pi} \left(\frac{N_A\,\rho}{M} \right) \right]^{1/3} v_m \tag{5}$$

where h is Plank's constants, k is Boltzmann's constant, N_A is Avogradro's number, ρ is the density, M is the molecular weight and n is the number of atoms in the molecule.

The average sound velocity v_m is given by

$$v_m = \left[\left[\frac{1}{3} \left(\frac{2}{v_t^{\,3}} + \frac{1}{v_l^{\,3}} \right) \right]^{-1/3} \right] \tag{6}$$

v_l and v_t are the longitudinal and transverse elastic wave velocities, respectively. These are obtained from the following expressions

$$v_l = \sqrt{\frac{3\,K\ +\ 4\,G}{3\,\rho}} \qquad \text{and} \qquad v_t = \sqrt{\frac{G}{\rho}} \tag{7}$$

where ρ is density, K is the bulk modulus and G is the shear modulus.

3. Results and Discussion

In order to calculate the value C_{ij}, one requires the values of force constants K_2. The values of K_2 are fixed with the values of C_{11} at room temperature [24-26]. The values of bulk moduli (K) for $x= 0.10$ to 0.20 at room temperature are evaluated with the help of computed values of SOE constants for all HTCS under study. Our computed values of bulk moduli for the tetragonal phase of $La_{2-x}Sr_xCuO_4$ provide new information about the structural phase transition (SPT) and doping attenuation.

We attribute differences in bulk moduli primarily to the formation of the orthorhombic phase. It is clear from Table 1 that the value of bulk moduli is decreasing with the increase of Sr doping. Doped material is stiffer than its undoped counterpart La_2CuO_4 [13].

The values of longitudinal elastic wave velocity (v_l) and transverse elastic wave velocity (v_t) and average (v_m) sound velocities in cm/s have been computed with the help of elastic data using Eqs. (6-7). The values are shown in Table 1 from which it is clear that

Table 1. Bulk modulus K_S, longitudinal (v_l), transverse (v_t) and average (v_m) sound velocities.

HTSC	K_s GPa	G GPa	v_l 10^5 cm/s	v_t 10^5 cm/s	v_m 10^5 cm/s
$La_{1.90}Sr_{0.10}CuO_4$	131.67	70.34	5.58	3.15	3.50
$La_{1.89}Sr_{0.11}CuO_4$	127.92	68.45	5.49	3.10	3.44
$La_{1.88}Sr_{0.12}CuO_4$	124.20	66.17	5.40	3.05	3.38
$La_{1.87}Sr_{0.13}CuO_4$	121.93	63.02	5.25	3.01	3.32
$La_{1.86}Sr_{0.14}CuO_4$	116.57	61.05	5.18	2.95	3.28
$La_{1.85}Sr_{0.15}CuO_4$	112.76	60.24	5.15	2.91	3.24
$La_{1.84}Sr_{0.16}CuO_4$	107.23	57.28	5.02	2.83	3.15
$La_{1.83}Sr_{0.17}CuO_4$	102.61	54.05	4.88	2.76	3.02
$La_{1.82}Sr_{0.18}CuO_4$	98.29	50.02	4.76	2.66	2.94
$La_{1.81}Sr_{0.19}CuO_4$	94.01	48.19	4.66	2.60	2.92
$La_{1.80}Sr_{0.20}CuO_4$	91.19	48.70	4.63	2.61	2.90

the values of longitudinal and transverse elastic wave velocities decrease with the increase of Sr doping and therefore the average sound velocity deceases. The computed velocities are used to obtain the value of Debye temperature (θ_D) for all the superconductors under study and are included in Table 2.

Table 2. Calculated values of θ_D, K_n-K_s and T_c.

HTSC	Θ_D (K)	K_n-K_s	T_C (K)
$La_{1.90}Sr_{0.10}CuO_4$	377.8	-17.87	29.5 (29.5)
$La_{1.89}Sr_{0.11}CuO_4$	371.4	-14.12	31.28
$La_{1.88}Sr_{0.12}CuO_4$	366.8	-10.4	33.3
$La_{1.87}Sr_{0.13}CuO_4$	364.3	-8.13	34.93
$La_{1.86}Sr_{0.14}CuO_4$	360.2	-2.77	36.7
$La_{1.85}Sr_{0.15}CuO_4$	350.0	1.04	38 (39)[a]
$La_{1.84}Sr_{0.16}CuO_4$	345.3	6.57	36.8
$La_{1.83}Sr_{0.17}CuO_4$	334.2	11.19	35.5
$La_{1.82}Sr_{0.18}CuO_4$	322.4	15.51	34.4
$La_{1.81}Sr_{0.19}CuO_4$	312.3	19.79	33.2
$La_{1.80}Sr_{0.20}CuO_4$	313.4	22.61	32 (32.6)

a-Expt. [15].

It is clear from Table 1 that the value of bulk modulus in superconducting phase (K_s) is larger than the value of bulk modulus in its normal phase (K_n=113.8 GPa) in the limit x=0.10 to x=0.14. After this limit K_s is lower than the value of bulk modulus in its normal phase (K_n=113.8 GPa). It is interesting to note that the value of (K_n-K_s) is minimum in case of $La_{1.85}Sr_{0.15}CuO_4$ whereas the value of T_c is high [15]. The superconducting phase transition at T_c is a second order transition which does not involve a change in density. Thus we suggest that (K_n-K_s) may be related with T_c as

$$K_n\text{-}K_s = \text{Const. } T_c \tag{8}$$

This empirical relation clearly shows the dependence of T_c on the difference of bulk modulus hence on the elastic constants of the HTSC. We tried to correlate the variation in transition temperature (T_c) and the difference in computed values of bulk modulus (K_n-K_s) of $La_{2-x}Sr_xCuO_4$ and the parent samples La_2CuO_4. The values of (K_n-K_s) are computed and are given in Table 2. Keeping in mind of this idea, a best fit figure is drawn with the help of known experimental values of T_c [15] and the computed values of (K_n-K_s) of $La_{1.90}Sr_{0.10}CuO_4$ and $La_{1.85}Sr_{0.15}CuO_4$.
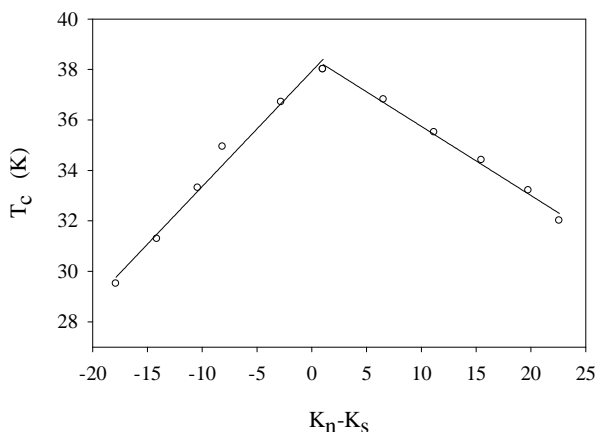

Fig. 1. T_c against difference of bulk moduli (K_n-K_s) for $La_{2-x}Sr_xCuO_4$.

The values of T_c are computed for the known values of (K_n-K_s) for all $La_{2-x}Sr_xCuO_4$ with the help of the proposed Fig. 1 and are shown in Table 2. It is interesting to note that from the Table 2 that the values of T_c decrease as the differences in (K_n-K_s) increase. The value for T_c of $La_{1.85}Sr_{0.15}CuO_4$ obtained with the help of Fig. 1 is maximum among all HTCS under study and is in good agreement with the experimental value [15].

The present features in the elastic constants near T_c may be important to the theory of the high temperature oxide superconductors. Many conventional (non-oxide) superconductors with high transition temperatures have transitions that are accompanied

by structural instabilities or structural transitions. In some cases the structural transition may be arrested by the onset of superconductivity, but the structural instability remains.

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