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Mechanism of the Dynamic Thermal Expansion of Bismuth-Based High-T_c Superconductors[1]

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The dynamic process of thermal expansion (DPTE) of Bi-based high-T_c (HTC) superconductor samples ($Bi_2Sr_2Ca_2Cu_3O_{10}$, $T_c = 105$ K) is studied theoretically. The abnormal expansion behavior in the superconducting and normal states are of relevance to the energy absorption and pairing mechanisms.

KEY WORDS: dynamic process of thermal expansion; energy absorption; high-T_c superconductors.

1. INTRODUCTION

Since the discovery of the high-T_c copper oxides, their thermal expansion properties have been widely studied [1–3], but all of these studies involved the steady-state thermal expansion process. The dynamic process of thermal expansion (DPTE) was first anticipated in 1986 by one of the authors [4], who considered it as an anharmonic and time-dependent process under the transient pulse heating condition.

In this paper, we study the mechanism of the abnormal expansion behavior of $Bi_2Sr_2Ca_2Cu_3O_{10}$ ($T_c = 105$ K), which has been observed experimentally by Guo et al. [5, 6]. Their result is given in Fig. 1, which shows typical evidence of the dynamic thermal expansion of the sample

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under the same heating energy (0.1 μs laser pulse heating) at different temperatures. It can be seen that under the same heating energy, the amplitude at $T < T_{c'}$ ($T_{c'} \simeq 100$ K) is almost one order of magnitude higher than that at $T > T_c$ ($T_c = 105$ K). Moreover, there is an obvious dynamic thermal expansion transition at a temperature close to T_c, and the amplitude increases sharply around T_c. The transition region is about 5 K. This behavior is quite different from that in steady-state thermal expansion. It is known that the latter shows little difference below and above the superconducting transition temperature T_c [1]. We wonder whether this anomaly is an important physical property of HTC superconductors, and whether it has some correlation to the mechanism of HTC superconductivity. To this end, theoretical considerations are presented in the next section. The discussion and concluding remarks are given in Sections 3 and 4.

2. THEORETICAL CONSIDERATIONS

According to the Grüneisen theory [7], the thermal expansion coefficient α is related to the specific heat C_v. Although there are anomalies in C_v–T and α–T curves near T_c, the jumps of C_v and α are only about 1% of the total value; they are not big enough to show an increase of almost one order of magnitude in the dynamic thermal expansion. Therefore, another theory must be used to account for the dynamic thermal expansion process.

We introduce ψ_1 and ψ_2 to denote the macroscopic quantum state wave functions of the phase-coherent superconducting state and phase-disordered normal state, respectively. We assume that there are two components of the carriers in both states; these are the paired and nonpaired carriers. The paired component is predominant in the superconducting state, whereas the nonpaired component is predominant in the normal state. We assume that the coupling between paired and nonpaired carriers is mainly determined by the paired component. Therefore, the coupling between paired and nonpaired carriers in the normal state is far weaker than that in the superconducting state. In an experiment, the sample is heated uniformly along the expansion direction (x direction), so we assume ψ_1 and ψ_2 are independent of x. We assume ψ_1 and ψ_2 satisfy the following Schrödinger equations:

$$i\hbar \frac{\partial \psi_1}{\partial t} = U_1 \psi_1 + K_1 \psi_1 \psi_2 \tag{1}$$

$$i\hbar \frac{\partial \psi_2}{\partial t} = U_2 \psi_2 + K_2 \psi_1 \psi_2 \tag{2}$$

where U_1 and U_2 are the energies of the superconducting and normal states, respectively, K_1 and K_2 are the coupling coefficients between paired and nonpaired carriers in the superconducting and normal states, respectively, and $K_2 \ll K_1$, $K_2 \ll U_2$. Let

$$\psi_1 = \sqrt{\rho_1}\, e^{i\varphi_1}$$
$$\psi_2 = \sqrt{\rho_2}\, e^{i\varphi_2}$$

where ρ_1 and ρ_2 denote the densities of carriers of the superconducting and normal states, respectively, and φ_1 and φ_2 are the phases of the two states, respectively. From Eqs. (1) and (2), we then have

$$\frac{\hbar}{2\sqrt{\rho_1}} \frac{\partial \rho_1}{\partial t} = K_1 \sqrt{\rho_1 \rho_2} \sin \varphi_2 \tag{3}$$

$$-\hbar \frac{\partial \varphi_1}{\partial t} = U_1 + K_1 \sqrt{\rho_2} \cos \varphi_2 \tag{4}$$

$$\frac{\hbar}{2\sqrt{\rho_2}} \frac{\partial \rho_2}{\partial t} = K_2 \sqrt{\rho_1 \rho_2} \sin \varphi_1 \tag{5}$$

and

$$-\hbar \frac{\partial \varphi_2}{\partial t} = U_2 + K_2 \sqrt{\rho_1} \cos \varphi_1 \tag{6}$$

From Eqs. (3) and (4), we have

$$\frac{\partial \rho_1}{\partial t} = \frac{-2\rho_1}{\hbar} \operatorname{tg} \varphi_2 \left(U_1 + \hbar \frac{\partial \varphi_1}{\partial t} \right) \tag{7}$$

From Eqs. (5) and (6), we have

$$\frac{\partial \rho_2}{\partial t} = \frac{-2\rho_2}{\hbar} \operatorname{tg} \varphi_1 \left(U_2 + \hbar \frac{\partial \varphi_2}{\partial t} \right) \tag{8}$$

$$= \frac{2K_2}{\hbar} \rho_2 \sqrt{\rho_1} \sin \varphi_1 \tag{9}$$

We hold that the superconducting state is the phase-coherent state; therefore, we assume φ_1 is time independent, i.e., $\varphi_1 = \text{const}$, and

$$\frac{\partial \varphi_1}{\partial t} = 0 \tag{10}$$

Since $K_2 \ll U_2$, from Eq. (6) we obtain

$$\varphi_2 \approx -\frac{U_2}{\hbar} t + C \tag{11}$$

where C is a constant. Substituting Eqs. (10) and (11) into Eq. (7), we get

$$\frac{\partial \rho_1}{\partial t} = \frac{-2\rho_1 U_1}{\hbar} \operatorname{tg}\left(-\frac{U_2}{\hbar} t + C\right) \tag{12}$$

From Eq. (12), we have

$$\sqrt{\rho_1} = C_1 \left[\cos\left(-\frac{U_2 t}{\hbar} + C\right)\right]^{-U_1/U_2} \tag{13}$$

where C_1 is a constant. Substituting Eq. (13) into Eq. (9), we have

$$\frac{\partial \rho_2}{\partial t} = \frac{2K_2\rho_2}{\hbar} C_1 \sin\varphi_1 \left[\cos\left(-\frac{U_2 t}{\hbar} + C\right)\right]^{-U_1/U_2} \tag{14}$$

According to the continuity equation, $\partial\rho/\partial t + \operatorname{div}(\rho\vec{v}) = 0$, where $\vec{v}$ is the velocity of the carriers. In our situation, the above equation leads to

$$\frac{\partial \rho}{\partial t} = -\rho \frac{\partial v_x}{\partial x} \tag{15}$$

Combining Eqs. (12), (14), and (15), we have

$$\frac{\partial v_{1x}}{\partial x} = \frac{2U_1}{\hbar} \operatorname{tg}\left(-\frac{U_2}{\hbar} t + C\right) \tag{16}$$

and

$$\frac{\partial v_{2x}}{\partial x} = \frac{-2K_2}{\hbar} C_1 \sin\varphi_1 \left[\cos\left(-\frac{U_2 t}{\hbar} + C\right)\right]^{-U_1/U_2} \tag{17}$$

We define the average velocity of the carriers as $\langle v_x \rangle = (1/L_0)\int_0^{L_0} v_x\, dx$, where L_0 is the original length of the sample. Then we get

$$\langle v_{1x} \rangle = \frac{L_0}{\hbar} U_1 \operatorname{tg}\left(-\frac{U_2}{\hbar} t + C\right) + C_2 \tag{18}$$

and

$$\langle v_{2x} \rangle = \frac{-L_0 \sin \varphi_1 C_1}{\hbar} K_2 \left[\cos\left(-\frac{U_2 t}{\hbar} + C \right) \right]^{-U_1/U_2} + C_3 \qquad (19)$$

where C_2 and C_3 are constants.

We suppose the paired carriers in superconductng states are a new kind of exciton to be determined. Our previous study [8] seemed to support a bipolaron mechanism. When the carriers move in the samples, they give rise to lattice polarizations and lattice displacements, and thus to expansion. From the point of view of the wave properties of the carriers, the propagations of the wave functions ψ_1 and ψ_2 lead to expansion. Therefore, concerning the thermal expansion, we believe that the abnormal behavior is derived from the time-dependent carrier distribution. Hence, we propose that the expansion of the sample is determined from $L = \int_0^\tau \langle v_x \rangle \, dt$, where τ is the characteristic time of the expansion, which is given by the experiment, and L is the length of the sample after expansion.

We finally get

$$\frac{L_1}{L_0} = \frac{U_1}{U_2} \ln \cos\left(-\frac{U_2 \tau}{\hbar} \right) + \frac{C_2 \tau}{L_0} \qquad (20)$$

where we have assumed $C = 0$. We assume $C_2 = 0$; then from Eq. (20), $U_1/U_2 < 0$. If $U_2 > 0$, then $U_1 < 0$. We have

$$\frac{L_2}{L_0} = \frac{-3\tau}{8} \frac{K_2 \sin \varphi_1 C_1}{\hbar} + \frac{3K_2}{16U_2} \sin \varphi_1 C_1 \sin\left(-\frac{2U_2 \tau}{\hbar} \right) + \frac{K_2}{4U_2} \sin \varphi_1 C_1 \sin\left(-\frac{U_2 \tau}{\hbar} \right) \cos^3\left(-\frac{U_2 \tau}{\hbar} \right) \qquad (21)$$

where we have assumed $C_3 = 0$, and $U_1/U_2 = -4$. Because $K_2 \ll U_2$, we have

$$\frac{L_2}{L_0} \approx \frac{-3\tau}{8} \frac{K_2 \sin \varphi_1 C_1}{\hbar} \qquad (22)$$

Then the expansions are given by $\Delta L_1 = L_1 - L_0$ and $\Delta L_2 = L_2 - L_0$.

According to the experiment, the transition region is from $T = 105$ K to $T = 100$ K, and the range is $\Delta T_c = 5$ K. On the basis of the assumption

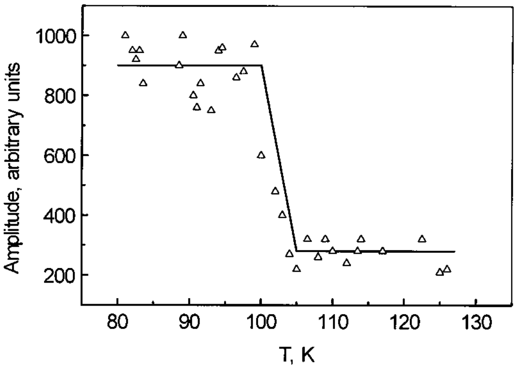

Fig. 1. Experimental data and theoretical curve for the dynamic thermal expansion amplitude of $Bi_2Si_2Ca_2Cu_3O_{10}$ sample ($T_c = 105$ K): ΔL (in arbitrary units) versus temperature T under the same laser pulse heating. Triangles represent experimental data, and the curve has been theoretically determined. $K_2 \sin \varphi_1 C_1/\hbar = -5.511 \times 10^4$, $\tau = 5.0 \times 10^{-5}$ s, $U_1/U_2 = -4$, and $-U_2\tau/\hbar = -0.7102 - 2\pi n$, where n is an integer.

that the thermal expansion in the transition region is the simple combination of those of two nontransition regions, we have

$$(\Delta L)_{\Delta T_c = 5\text{ K}} = m_1(T)\,\Delta L_1 + m_2(T)\,\Delta L_2 \tag{23}$$

We have $m_1(T) = (105 - T)/\Delta T_c$, and $m_2(T) = (T - 100)/\Delta T_c$.

Equations (20), (22), and (23) are plotted in Fig. 1, and are in good agreement with experiment.

3. DISCUSSION

According to Eq. (20), in the superconducting state, the expansion scale is proportional to the energy of the superconducting state and inversely proportional to that of the normal state. Thus, for the same sample under the same heating energy, the large expansion amplitude in the superconducting state originates from the large energy absorption compared to the normal state. Compared to the steady-state thermal expansion, which exhibits little difference below and above the superconducting transition temperature T_c [1], we suppose that the sample in the superconducting state tends to absorb much more energy in the dynamic heating condition than that in the steady-state heating condition. We think this is an inherent property of the HTC superconductors, which may be of relevance to the mechanism of HTC superconductivity. It thus appears that the anomaly of the dynamic thermal expansion may be related to the superconductivity. This theory could not give this energy absorption mechanism due to the neglect of the detailed microscopic energy transfer process. Nevertheless, it suggests that the superconducting and normal states have quite different energy absorption mechanisms.

According to Eq. (22), the expansion amplitude in the normal state is proportional to the coupling coefficient K_2 between paired and nonpaired carriers. Thus, the small expansion in the normal state may be due to the reason that there are few paired carriers. On the contrary, in the superconducting state, there are large quantities of paired carriers, which causes large expansion. Therefore, we anticipate that the energy absorption and the expansion behavior seem to be related to the carrier pairing.

According to Eq. (20), we assume $U_1 < 0$ and $U_2 > 0$. This means that in the superconducting state the energy can be negative, which leads to the formation of the paired carriers. Indeed, when the static dielectric constant is quite large or some additional attractive energy mechanism is present, bipolaron formation would occur [9]. An additional attractive mechanism may be provided by the magnetic exchange energy. There are experiments that demonstrate the bipolaron mechanism [10].

According to experiment, the expansion amplitudes are nearly independent of temperature in both states near T_c (neglecting the disturbances in the experimental data, which originate from the unstable factors, e.g., input laser power is not absolutely stable). Therefore, we have not considered the temperature dependences of the energies in these states.

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