Hysteretic behavior of the thermal conductivity in $YBa_2Cu_3O_{7-\delta}$

A. P. Saĭko, V. E. Gusakov, and V. S. Kuz'min
Institute of Solid State and Semiconductor Physics, Academy of Sciences of Belarus, 220726, Minsk, Belarus

(Submitted 16 December 1992)
Pis'ma Zh. Eksp. Teor. Fiz. **57**, No. 2, 108–111 (25 January 1993)

The hysteresis seen experimentally in the thermal conductivity of both superconducting and nonsuperconducting $YBa_2Cu_3O_{7-\delta}$ is explained in terms of a bistable behavior of the sublattice of O(4) apical oxygen atoms.

1. It was recently shown[1] that the existence of a bistable sublattice consisting of apical oxygen atoms in the $YBa_2Cu_3O_{7-\delta}$ system may lead to high superconducting transition temperatures on the basis of the standard electron–phonon pairing mechanism.

In this letter we wish to show that the hysteretic behavior of apical oxygen atoms makes it possible to offer a theoretical explanation for certain experimental facts which have heretofore seemed puzzling. We are talking primarily about precise measurements[2,3] of the thermal conductivity of the $YBa_2Cu_3O_{7-\delta}$ system with $\delta=0$–1. It has been found that there is a hysteresis in the thermal conductivity over a broad temperature range, 80–240 K, in both superconducting and nonsuperconducting samples of $YBa_2Cu_3O_{7-\delta}$. Since this anomalous behavior is not seen in the electrical resistance, and since the electron component of the thermal conductivity is comparatively small, Jezowski *et al.*[2,3] concluded that the hysteresis was not due to the electron component and was instead the result of an instability of the phonon subsystem.

2. Under the assumption that such anomalies in the thermal conductivity are a consequence of a bistability of the sublattice formed by the O(4) apical oxygen atoms, we can find the corresponding component of the lattice thermal conductivity **k** (Ref. 4):

$$k(T)=\frac{1}{3}c_v u\Lambda, \tag{1}$$

where u and Λ are the mean velocity and mean free path, respectively, of the phonons, and c_v is the specific heat at constant volume. As in Ref. 1, we treat the sublattice of O(4) atoms as a system of interacting anharmonic oscillators, each of which is moving in a bistable potential. If the interaction between oscillators is a long-range dipole interaction, the binary force coefficients f_{ij} can be approximated as $f_{ij}=f/N$, where N is the number of unit cells, and the indices i, j run over all the cells. Our model for a single collective degree of freedom—vibrations of the O(4) atoms along the crystallographic c axis—then reduces to a one-particle problem, with the effective lattice Hamiltonian

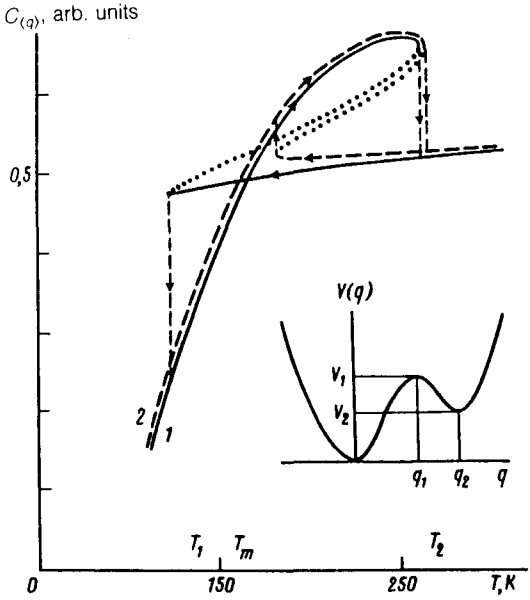

FIG. 1. Temperature dependence of the specific heat $c_{\langle q\rangle}$ calculated from (7). The dotted lines are unstable branches. The inset shows the one-particle potential for an O(4) apical oxygen atom, $V(q)=\alpha q^2/2-\beta q^3/3+\gamma q^4/4$. The parameters of the potential were chosen as in Ref. 1. *1*—$V_1=0.038$ eV, $q_1=0.054$ Å, $v_2=0.0036$ eV, $q_2=0.106$ Å; 2—0.038, 0.057, 0.0126, 0.106 ($f=0.01\alpha$).

$$H(p,q)=\frac{p^2}{2m}+\frac{\alpha+f}{2}q^2-\frac{\beta}{3}q^3+\frac{\gamma}{4}q^4-f\langle q\rangle q, \tag{2}$$

where q and p are the canonically conjugate coordinate and momentum of the anharmonic oscillator in the mean field $f\langle q\rangle$, and the angle brackets mean a quantum-statistics expectation value with Hamiltonian (2). Making the substitution $q\to\langle q\rangle+\delta q$ in (2), and using the approximation[5] of self-consistent phonons [$\langle(\delta q)^{2n}\rangle=(2n-1)...3\sigma^n$, $\langle(\delta q)^{2n+1}\rangle=0$, and n is an integer], we find the energy expectation value $E=\langle H(p,\delta q)\rangle$:

$$E=\frac{\alpha+f}{2}\langle q\rangle^2-\frac{\beta}{3}\langle q\rangle^3+\frac{\gamma}{4}\langle q\rangle^4-f\langle q\rangle^2+\Omega^2\sigma-\frac{3}{4}\gamma\sigma^2. \tag{3}$$

Here $\langle q\rangle$ and $\sigma=\langle q^2\rangle-\langle q\rangle^2$ are determined in a self-consistent way from the system of equations[1]

$$\sigma=(\hbar/2m\Omega)\coth(\hbar\Omega/2\theta), \tag{4}$$

$$(\beta-3\gamma\langle q\rangle)\sigma=\alpha\langle q\rangle-\beta\langle q\rangle^2+\gamma\langle q\rangle^3, \tag{5}$$

$$\Omega^2\equiv[\alpha+f-2\beta\langle q\rangle+3\gamma(\sigma+\langle q\rangle^2)]/m, \quad \theta=k_BT. \tag{6}$$

We write the specific heat at constant volume (at a constant average displacement $\langle q\rangle$) per particle as

$$c_{\langle q\rangle}=k_B\left(\frac{\partial E}{\partial\theta}\right)_{\langle q\rangle}=k_B\frac{m\Omega^2(3\gamma\sigma+2m\Omega^2)(4m^2\Omega^2\sigma^2-\hbar^2)}{\theta[8\theta m^2\Omega^2+3\gamma(4m^2\Omega^2\sigma+4\theta m\sigma-\hbar^2)]}. \tag{7}$$

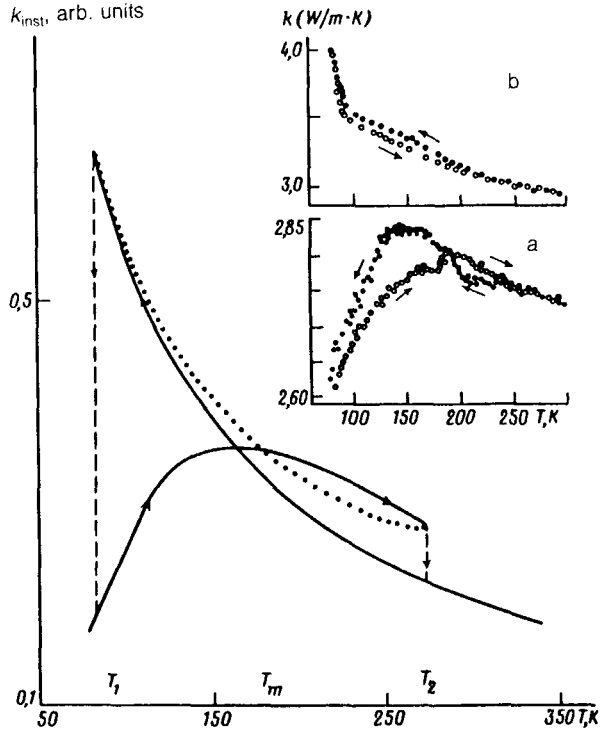

FIG. 2. Theoretical temperature dependence of the thermal conductivity k_{inst} of a bistable sublattice consisting of O(4) apical oxygen atoms in the compound $YBa_2Cu_3O_{7-\delta}$. The dots show an unstable branch. The insets show experimental results[2,3] on the temperature dependence of the thermal conductivity of $YBa_2Cu_3O_{7-\delta}$. *a*—A nonsuperconducting sample ($\delta \approx 1$); *b*—a superconducting sample ($\delta \approx 0$).

If we now set[4] $u = \text{const}$ and $\Lambda \sim T^{-1}$ in (1), the component of the thermal conductivity corresponding to the anharmonically unstable lattice can be estimated from

$$k_{inst} \sim c_{\langle q \rangle} T^{-1}. \tag{8}$$

3. The specific heat constructed from (7) has a hysteresis (Fig. 1). This hysteresis curve changes shape, depending on the shape of the potential in which the O(4) atom is moving. Specifically, the hysteresis curve has a single loop if one of the minima is metastable, while it has two loops if the metastable minimum descends in such a way that the potential becomes essentially symmetric. At temperatures T_1 and T_2 the specific heat $c_{\langle q \rangle}$ has a finite discontinuity. This discontinuous behavior of the theoretical curves is smoothed over when the decay of the lattice mode of interest is taken into account.

Figure 2 shows the behavior of the thermal conductivity k_{inst}. Insets *a* and *b* show experimental results from Refs. 2 and 3. The nature of the hysteretic behavior—the two loops, the temperature interval (T_1, T_m, T_2), and the direction in which the

hysteresis loop is traced out—for the nonsuperconducting $YBa_2Cu_3O_{7-\delta}$ sample[2] (inset *a*) is conveyed completely, at a qualitative level, by the theoretical curve. The positions of the T_1, T_m, and T_2 points and also the shape of the curve are very sensitive to the parameters of the potential.

A hysteresis curve with a single loop is seen experimentally for the superconducting system (inset *b*). Theoretically, a curve of this sort can be derived by varying the parameters of the potential (in practice, this can be done by changing, say, δ). If one of the minima of the potential is metastable, the curve of the thermal conductivity acquires a single loop. However, (first) this loop lies in a different interval, namely, $T_m < T < T_2$. Second, in this case the hysteresis loop is traced out in the direction opposite that which is actually observed[3] (see the discussion of the specific heat above, and see the insets in Fig. 2). On the other hand, when we note that the difference between the values of the thermal conductivity for the heating and cooling curves decreases by a factor of 2 or 3 for the superconductor,[3] we can apparently conclude that a loop in the interval $T_m < T < T_2$ is simply not being resolved, and all that is being seen experimentally is the loop at $T_1 < T < T_m$. The characteristic shape of this loop and the higher thermal conductivities can be explained on the basis of an electron component which increases sharply near T_1.

The situation which prevailes in superconducting and nonsuperconducting $YBa_2Cu_3O_{7-\delta}$ is apparently one in which apical oxygen atoms are in a potential with two metastable minima (two nearly equivalent states). In other words, a variation of δ in the formula $YBa_2Cu_3O_{7-\delta}$ results in only a comparatively slight change in the shape of the potential and in its position.[6]

It can thus be said that the hysteresis of the thermal conductivity in superconducting and nonsuperconducting compounds of the $YBa_2Cu_3O_{7-\delta}$ type in the temperature range 80–240 K stems from a hysteretic behavior of the sublattice consisting of O(4) apical oxygen atoms.

This work was financed by the Fundamental Research Fund of Belarus.

[1] A. P. Saĭko, V. E. Gusakov, and V. S. Kuz'min, Pis'ma Zh. Eksp. Teor. Fiz. **56**, 425 (1992) [JETP Lett. **56**, 411 (1992)].
[2] A. Jezowski, J. Klamut, R. Horyn, and K. Rogacki, Supercon. Sci. Technol. **1**, 296 (1989).
[3] A. Jezowski, Solid State Commun. **71**, 419 (1989).
[4] H. J. Goldsmid (editor), *Problems in Solid State Physics*, Academic, New York, 1968.
[5] N. M. Plakida, in *Statistical Physics and Quantum Field Theory* (ed. N. N. Bogolyubov), Nauka, Moscow, 1973.
[6] D. Mihailovic and C. M. Foster, Solid State Commun. **74**, 753 (1990).

Translated by D. Parsons