Analysis of in-plane thermal conductivity anomalies in YBa$_2$Cu$_3$O$_{7-\delta}$ cuprate superconductors

Dinesh Varshney$^{1,4}$, K K Choudhary$^2$ and R K Singh$^3$

1 School of Physics, Vigyan Bhawan, Devi Ahilya University, Khandwa Road Campus, Indore 452017, India
2 Department of Physics, SVITS, Sanwer Road, Indore 453331, India
3 MP Bhoj (Open) University, Shivaji Nagar, Bhopal 462016, India
E-mail: vdinesh33@rediffmail.com and dvsbobson.sop@dauniv.ac.in

New Journal of Physics 5 (2003) 72.1–72.17 (http://www.njp.org/)
Received 13 March 2003
Published 16 June 2003

Abstract. A theoretical model is developed to account for the anomalies reported for the thermal conductivity ($\kappa$) of the high-$T_c$ YBa$_2$Cu$_3$O$_{7-\delta}$ cuprate superconductors. We begin with the lattice thermal conductivity by incorporating the scattering of phonons with defects, grain boundaries, tunnelling states, charge carriers and phonons in the model Hamiltonian. The lattice thermal conductivity dominating in this cuprate is an artifact of strong phonon defects, tunnelling states and the impurity scattering mechanism below $T_c$. Later on, the scattering of electrons with impurities is investigated in order to assess their role in thermal conduction. We also look for the spin-wave (magnon) contribution for thermal conductivity. It is noticed that at very low temperatures ($T < 10$ K), $\kappa$ increases and shows an almost $T^2$ dependence on the temperature, and is attributed to spin-wave thermal transport. Further, at 60 K, $\kappa$ develops a broad peak and then decreases as the temperature is increased. The anomalies are well accounted for in terms of interaction between the phonon impurity and the carrier impurity. We conclude that the behaviour of the thermal conductivity is determined by competition among the several operating scattering mechanisms for the heat carriers and a balance between electron, magnon and phonon contributions. Numerical analysis of thermal conductivity from the present model shows results similar to those revealed from experiments.

$^4$ Author to whom any correspondence should be addressed.
1. Introduction

The pairing mechanism and thermal transport of high-$T_c$ cuprate superconductors remain elusive in spite of the fact that many models have been proposed since their discovery. A fundamental question in cuprates is associated with the two-dimensionality of metal oxide layers and poses the possibility that these cuprates may be radically different from conventional metals. In order to clarify the issue of anomalous physical properties, several theories have been put forward, ranging through minor variations on the phonon based Bardeen–Cooper–Schrieffer (BCS) [1] mechanism and both strong- and weak-coupling theory [2]. Obviously, these approaches yield the high $T_c$ found in the oxide superconductors but differ in their predictions for other characteristic properties, in particular of the normal-state transport. The thermal conductivity $\kappa$ is non-zero in both normal and superconducting states and hence a good probe for electron and phonon systems in both. Unfortunately, most of the available experimental data vary sufficiently from technique to technique to convincingly confirm or rule out any approach.

In cuprates, such as, YBa$_2$Cu$_3$O$_{7-\delta}$, the exact mechanism of binding holes as carriers into Cooper pairs with high $T_c$ is still a matter of great debate. Furthermore, the pairing symmetry in cuprate superconductors is an important and much debated issue [3]. Much of the recent attention has been focused on a particular state with d-wave symmetry, the $d_{x^2-y^2}$ pairing state. Numerous studies have shown that normal-state properties deviate from a conventional Fermi liquid and as a possible explanation several workers proposed the antiferromagnetic correlations as responsible for such unconventional behaviour. The mechanism responsible for the superconducting state of high-$T_c$ superconductors is still discussed with high intensity. Since the announcement of cuprate superconductors, a growing list of theoretical models based on experimental results exists. It is now felt that d-wave symmetry is implied by a number of possible superconducting pairing mechanisms, particularly those involving magnetic interactions.

The establishment of d-wave pairing symmetry in high-$T_c$ cuprates does not necessarily specify a high-$T_c$ mechanism. It does impose constraints on possible models for this mechanism. While the spin fluctuation pairing mechanism leads naturally to an order parameter with d-wave pairing symmetry, the conventional BCS electron–phonon coupling pairing interaction yields s-wave superconductivity [1]. For the high-$T_c$ superconductors there is a very interesting large group activity for a pairing model [2, 3] involving substances with phonons, polarons and bipolarons, excitons, charge density fluctuation, spin density fluctuation, magnons and resonating bond states. Nevertheless, the BCS theory and the Cooper pairing concept remain the cornerstone.
of almost all current theories of superconductivity. Recently, we have developed an approach based on the screening of phonons with charge density fluctuation in an area where local AF order exists inducing d-wave superconductivity in cuprates [4].

The thermal conductivity of superconductors seems to be an interesting transport phenomenon and is still discussed with high intensity for high-$T_c$ superconductors. It is worth mentioning the pioneering work of the Bardeen–Rickayzen–Tewordt (BRT) theory of thermal conductivity ($\kappa$) on the basis of the BCS formalism [5]. The BRT theory exactly calculates the electronic contribution to thermal conductivity when the dominant scatterers are impurities as well as the effect of electrons on the thermal conductivity of conventional superconductors. Morelli et al [6] have reported the temperature-dependent thermal conductivity behaviour of YBa$_2$Cu$_3$O$_{7-\delta}$ and argued that the nearly temperature-independent $\kappa$ above $T_c$ together with the sharp rise in $\kappa$ below $T_c$ indicates a strong electron–phonon interaction in the normal state. Uher and Kaiser ascribe the sharp increase in $\kappa$ below $T_c$ to an increase in the lattice conduction due to a reduction in the scattering of phonons by holes as superconducting pairs form in YBa$_2$Cu$_3$O$_{7-\delta}$ [7]. On the other hand, Nunez Regueiro et al [8] propose formation of polaronic or bipolaronic glass in cuprates such as the La–Sr–CuO system due to oxygen vacancies. The random vacancy distribution leads to the formation of a two-level system, which relaxationally scatters phonons at low temperatures. The understanding of these measurements [6]–[8] for $\kappa$ on cuprates leads to an insight that the phonon contribution plays an important role and the thermal current is mainly carried by phonons.

Phonons are important in an ionic lattice such as YBa$_2$Cu$_3$O$_{7-\delta}$ and inelastic neutron scattering measurements [9], as well as Raman scattering of light [10], have been employed to probe its phonon structure. The features in the phonon spectrum indicate the strong coupling of the phonons to the electrons as carriers in the CuO$_2$ planes. It remains to be seen whether they play a substantial role in the thermal transport. In this regard, thermal conductivity measurements are an indispensable tool. Since heat is carried by both charge carriers and by phonons, a measurement of the thermal conductivity can yield valuable information not only about phonons and carriers and the interaction between them but also about the impurities in the system. It is worth pointing out that, in most cases, explanation of experimental results is complicated because both the carriers and the phonons contribute to the thermal conduction and perhaps most important is the fact that both contributions are limited by several scattering mechanisms. We now turn to the reported temperature dependence of thermal conductivity behaviour in YBa$_2$Cu$_3$O$_{7-\delta}$ superconductors.

Salient features reported for the thermal conductivity ($\kappa$) follow:

(1) in the low-temperature domain ($0.1 < T < 10$) $\kappa$ exhibits a clear $T^2$ dependence on the temperature,

(2) at a temperature around 60 K $\kappa$ develops a broad peak and

(3) at higher temperatures $\kappa$ is independent of temperature and also decreases with a change of the slope [11, 12].

The quadratic temperature dependence at low temperature as well the origin of the peak at the critical temperature is still unclear and is reviewed at great length. The characteristic peak structure has been described as being due to the contribution of normal electrons in the CuO$_2$ plane [13]. Further, in YBa$_2$Cu$_3$O$_{7-\delta}$, Cu atoms are magnetic and at low temperatures the magnetic ordering of the Cu atoms must have a strong impact on the thermal conductivity. As a consequence, the spin-wave contribution for thermal transport at low temperatures is important
in this test material. We may recall the theoretical calculation by Mikhail [14], which suggests the involvement of spin-waves for the consistent explanation of $\kappa$ of La$_2$CuO$_{4+\delta}$.

We may also refer to the earlier work of Houssa et al [15], who have interpreted the temperature dependent $\kappa$ of YBa$_2$Cu$_3$O$_{7-\delta}$ with the help of an electronic model, i.e., supposing that the main contribution to $\kappa$ below $T_c$ is due to electron scattering in the CuO$_2$ plane. Following the two-fluid model derived from the kinetic theory the authors obtain the theoretical curves which reproduce the experimental results. They properly incorporate the temperature dependence of the electronic relaxation time and the normal charge carrier concentration. Hirschfeld and Putikka [16] have calculated the thermal conductivity of Y–Ba–CuO, including the effect of impurity scattering and inelastic scattering by antiferromagnetic spin fluctuations, and argue that phonons dominate heat transport near $T_c$, but the electrons are responsible for most of that observed in clean samples. In trying to understand the interplay between electrons, phonons, fluctuations and magnons, several reports have appeared where experimental data and theoretical aspects of $\kappa$ of high-$T_c$ superconductors are reviewed [17].

While explaining the anomalies observed in the thermal conductivity, we first need to understand the interplay of scattering processes between the heat carriers themselves and between the carriers and the impurities, the tunnelling states etc. The thermal conductivity behaviour of La–Sr–CuO shows the importance of phonon scattering tunnelling systems analogous to those found in glasses [11, 18]. The anomalous linear $T$ term in the specific-heat measurements and the $T^2$ dependence of $\kappa$ are hallmarks of the existence of tunnelling states in amorphous materials [19, 20]. Such behaviours have been well documented for cuprates by acoustic methods [21]. Also, it is important to look for the relative magnitudes of these scattering process which lead to the anomalous behaviour, and this motivates us for the present investigation. It is obvious that the thermal conductivity depends on the way the heat carriers interact with one another and with the environment. The results we report here do indeed shed some very important light on the nature of phonon, electronic and spin-wave components of $\kappa$ in the test material.

In order to obtain numerical results, we will work with a model Hamiltonian within the relaxation time approximation to estimate the phonon contribution towards the thermal conduction incorporating the interactions of phonons with defects, electrons as carriers, grain boundaries and phonon–phonon interactions respectively. Later on, the role of electron–impurity scattering effects and magnon contribution at low temperature and zero magnetic field in the thermal conduction process is investigated. We find that the anomalies can be well accounted for through the use of the Debye model and a BCS-like model. Section 2 is devoted to the estimation of various scattering rates for the calculation of lattice, carrier and spin-wave thermal conductivity. In section 3, we return to a discussion of results and various plots are presented. A summary and our main conclusions are given in section 4.

2. The model

We start by giving a brief description of the high-$T_c$ superconductor YBa$_2$Cu$_3$O$_{7-\delta}$. YBa$_2$Cu$_3$O$_{7-\delta}$ is the best characterized and the most studied of the high-$T_c$ superconductors, since good crystals with a very sharp superconducting transition at $T_c$ can be prepared. The dimensions of the unit cell are approximately 12 and 4 Å in the $c$- and $a$- or $b$-axis directions respectively. However, it is by no means the simplest system as it contains a quasi-one-dimensional (1D) CuO chain layer (along the $b$-axis of the orthorhombic crystal structure and also regarded as the charge reservoir), two cuprate CuO$_2$ planes (parallel to the $ab$ plane approximately $\sim$3.2 Å apart, separated by yttrium ions), two BaO planes and Y.
The structure consists of a sequence of metal oxide layers perpendicular to the c-axis: in particular, the CuO layer in which the Cu (1) site has coordination 4 and is surrounded by four oxygen ions, which is the plane made by the CuO chains, and secondly the CuO layer in which Cu (2) has a coordination number 5 and is surrounded by five oxygen ions which form a polyhedron. This is the plane that we call the CuO2 plane. Further copper can be found at two different sites: Cu (1) within CuO4 squares and Cu (2) within a square-based pyramid, CuO5. In the crystal, yttrium is in the valence state Y3+, while barium is in the state Ba2+. Copper on the planes is Cu2+, and oxygen is O2−.

In YBa2Cu3O7−δ, the linear chain oxygen atoms are mobile and a percentage of the oxygen atoms may tunnel, providing the relevant low-energy excitations for this system at low temperatures. As mentioned earlier, the tunnelling systems have been experimentally observed in YBa2Cu3O7−δ by acoustic methods at low temperature [21]. Further, the extended x-ray-absorption fine-structure (EXAFS) spectra indicate a double well as a consequence of two Cu–O (4) distances [22]. We may also refer to an earlier work in which it has been shown that the electrons provide a double-well potential for the atom, which hops back and forth between the minima of tunnelling systems [23].

It is known that the high-$T_c$ superconductors, in particular YBa2Cu3O7−δ, have very complicated electronic structures. A first-principles calculation of the thermal conductivity requires a detailed knowledge of both the hole and phonon bands in addition to the working attractive pairing mechanism between a pair of carriers. We follow a simple model where the phonons are described in the Debye model and the carriers (holes) are treated in an isotropic BCS-like model. The use of the Debye model is reasonable since the temperature region of interest lies well below the Debye temperature. As the simplest approximation to the problem at hand, the isotropic BCS-like model can be used to derive qualitative results, as we will demonstrate below.
We start with a model Hamiltonian that follows [24]

\[ H = \sum_k \varepsilon_k a_k^+ a_k + \sum_q \omega_q b_q^+ b_q + \sum_{i=1,2} \varepsilon_i c_i^+ c_i + \sum_{k_1, k_2} \varphi(k_1, k_2) a_{k_1}^+ a_{k_2} \\
+ D_p \sum_{k, q} \left[ \frac{\hbar}{2 \rho \omega_q} \right]^{1/2} a_{k+q}^+ a_k (b_k + b_{-k}^+) + \frac{R}{2N} \sum_{q_1, q_2} \epsilon_i^{(q_1+q_2)j} \left[ \frac{\hbar \omega_{q_1} \omega_{q_2}}{4} \right]^{1/2} \\
\times (b_{q_1} - b_{-q_1}^+) (b_{q_2} - b_{-q_2}^+) + \sum_{q, i, j = 1, 2} \gamma_{ij} \left[ \frac{\hbar}{2 \rho \omega_q} \right]^{1/2} c_i^+ c_j (b_q + b_{-q}^+) + H_{ph-ph} \tag{1} \]

Here, the initial three terms are holes as carriers, phonons and two-level tunnelling-system excitation. The fourth and fifth terms represent the carrier–impurity interactions and carrier–phonon interactions, respectively. The sixth and seventh terms denote the phonon–impurity interactions and phonon–two-level tunnelling-system interaction, respectively. The last term represents the phonon–phonon interaction.

The notations \( a \) (\( a^+ \)), \( b \) (\( b^+ \)) and \( c \) (\( c^+ \)) are the creation (annihilation) operators for phonons, holes and tunnelling states. \( D_p \) is the deformation-potential constant. \( R \) is the relative ionic-mass difference ((\( M'' - M \))/\( M'' \)); \( \gamma \) and \( \phi \) are the coupling parameters of the two-level tunnelling system to the lattice vibration and the impurity potential, respectively. The phonon frequency of a wavevector \( q \) is \( \omega_q \). \( N \) is the number of cells. \( \rho \) is the mass density of ions and \( R_i \) stands for the position of defects. \( \varepsilon_k \) is the hole free energy. We begin our description with the phonon contribution to the thermal conduction.

### 2.1. Lattice (phonon) contribution

The thermal conductivity following the model Hamiltonian (equation (1)) can be calculated from the Kubo formula [25]. It has contributions from both the phonons and the carriers. We first explore the lattice part; in the continuum approximation

\[ \kappa_{ph} = \frac{k_B \hbar^2}{2 \pi^2 v_s} \int_0^{\omega_D} \frac{d\omega \omega^2 \tau(\omega)(\beta \omega)^2}{(\omega^2 - \beta^2)^2} \tag{2} \]

where \( k_B \) is the Boltzmann constant, \( v_s \) is the sound velocity, \( \omega_D \) is the Debye frequency and \( \beta = \hbar/k_B T \). The relaxation time is proportional to the imaginary part of the phonon self-energy. In the weak-interaction case, it has been calculated to the lowest order of the various interactions. The relaxation times are expressed as

\[ 1/\tau(\omega) = 2|\text{Im} \, P(\omega/v_s, \omega)| = 1/\tau_{ph-d} + 1/\tau_{ph-e} + 1/\tau_{ph-ts} + 1/\tau_{ph-gb} + 1/\tau_{ph-ph}, \tag{3} \]

with the various relaxation times defined as

\[ \tau_{ph-d}^{-1}(\omega) = (A/k_B^3) \omega^4 \hbar^3, \tag{4} \]
\[ \tau_{ph-e}^{-1}(\omega) = B \omega n_F(\Delta), \tag{5} \]
\[ \tau_{ph-ts}^{-1}(\omega) = P \omega \tanh(\beta \omega/2), \tag{6} \]
\[ \tau_{ph-gb}^{-1}(\omega) = v_s/L, \tag{7} \]
\[ \tau_{ph-ph}^{-1}(\omega) = C(T \omega \hbar/k_B)^3 \tag{8} \]

where \( L \) is the sample size, \( n_F \) is the Fermi–Dirac distribution function and \( \Delta \) is the gap function. The notation \( \tau_{ph-d} \), \( \tau_{ph-e} \), \( \tau_{ph-ts} \), \( \tau_{ph-gb} \) and \( \tau_{ph-ph} \) are the phonon scattering relaxation times.

New Journal of Physics 5 (2003) 72.1–72.17 (http://www.njp.org/)
due to defects, carriers, tunnelling states, grain boundaries and phonon–phonon interactions respectively. We note that to this order Mathiessen’s rule holds, namely, that the inverse of the total relaxation time is the sum of the various contributions for the different scattering channels.

Further, we define

\[ A = \left[ \frac{3n_i R^2}{4 \theta_{1p}} \right], \quad B = \frac{9\pi}{4} \left[ \frac{m}{3M} \right]^{1/2} \frac{D_\rho^2}{\varepsilon_F^2} \quad \text{and} \quad P = \frac{\pi n_{ts} \gamma^2}{2 \rho v_F^2}, \]  

(9)
as parameters which characterize the strengths of the phonon–defect, phonon–carrier and phonon–tunnelling state scattering processes. Here, \( n_i \) is the density of impurities or defects, \( \varepsilon_F \) is the Fermi energy of holes as carriers, \( m \) is their mass and \( n_{ts} \) is the density of tunnelling states. We shall proceed to include the effect of electrons as the carrier contribution to the thermal conductivity in the next sub-section.

2.2. Carrier contribution

The in-plane electronic thermal conductivity of the \( d_{x^2-y^2} \) wave superconductors for the low-temperature behaviour for the electron–impurity contribution [26] is

\[ \lim_{T \to 0} \kappa_{e-i} = \frac{\hbar}{2m} k_B \varepsilon_F \left( \frac{\pi}{d} \right) N^{-1} \left( \frac{Z e^2}{\varepsilon_c} \right)^{-2} \left( \frac{k_B T}{\Delta(0)} \right)^2, \]  

(10)
with \( N \) the impurity fraction in the sample, \( \varepsilon_c \) being the high-frequency background dielectric constant, \( \varepsilon_F \) the energy at the Fermi level and \( d \) the inter-planar distance.

2.3. Spin-wave contribution

In YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) superconductors, the magnetic ordering of Cu atoms has a strong effect on thermal transport, in particular the thermal conductivity. This effect is sensitive to an applied magnetic field. The two-dimensional structure of test material allows the existence of 2D antiferromagnetic spin-wave excitations. Thus, we believed that spin-wave excitations would be an additional source of thermal transport in the test material.

At low temperature, particularly in the liquid-helium range, magnons contribute significantly to the thermal conductivity in a magnetic crystal. A calculation of the magnon thermal conductivity has been proposed by Douthett and Friedberg [27] in a way analogous to the calculation of the phonon thermal conductivity. The dispersion relation of a spin-wave of wavenumber \( k \) follows

\[ \hbar \omega_k = Dk^2 + g\mu H, \]  

(11)
where \( D \) is the constant proportional to the exchange energy, \( g \) is the spectroscopic splitting factor and \( \mu \) the Bohr magneton. For appropriate crystalline directions, \( H \), as used in this expression, may be regarded as the resultant of an external field and an anisotropy field. If one assumes an effective magnon mean free path, \( l_s \) independent of \( k \) (wavenumber), then this expression yields for the spin-wave thermal conductivity at low temperatures

\[ \kappa_m = \frac{l_s k_B^3 T^2}{3\pi \kappa D} \sum_{n=1}^\infty \left[ \left( \frac{g\mu H}{k_B T} \right) \frac{1}{n} + \left( \frac{4g\mu H}{k_B T} \right) \frac{1}{n^2} + \frac{6}{n^3} \right] \exp \left( \frac{-n\mu g H}{k_B T} \right), \]  

(12)
which for \( H = 0 \) reduces to

\[ \kappa_m = \frac{0.765 l_s k_B^3 T^2}{\hbar D}. \]  

(13)
We shall now estimate and compute numerically the phonon, electron and magnon contributions to the thermal conductivity as well the effects of different scattering mechanisms in the following section.

3. Results and discussion

In the calculation of temperature-dependent thermal conduction of YBa$_2$Cu$_3$O$_{7-\delta}$, we use the following parameters to characterize the strengths of the phonon–tunnelling state, phonon–defect, phonon–carrier and phonon–phonon scattering processes: $A = 4.9 \times 10^{-8}$ K$^{-3}$, $B = 1.47 \times 10^{-3}$, $P = 2.45 \times 10^{-3}$, and $C = 0.3$ K$^{-6}$ s$^{-1}$ respectively. These are indeed free parameters for phonon thermal transport in the present model. The length of the sample is about 3 mm and $v_s = 7 \times 10^5$ cm s$^{-1}$. In the model Hamiltonian, we presume that the high-$T_c$ YBa$_2$Cu$_3$O$_{7-\delta}$ superconductors contain the tunnelling states, the defects, the phonons and the BCS-like quasi-particles, interacting with one another. Thus, in the following discussions, we begin the phonon channel of thermal transport.

Let us first discuss the relative magnitudes of the various scattering mechanisms. A plot of various scattering phonon relaxation times as a function of $x (=\hbar \omega/k_BT)$ in terms of frequency at $T = 20$ K from equation (2) is shown in figure 2. It can be seen that the phonon–tunnelling state scattering dominates the phonon–defect scattering at low frequencies while the reverse is true at high frequencies. Similar features are revealed at different temperatures (40, 80 and 100 K) as shown in figures 3–5 i.e., in the normal and superconducting states. At a temperature $T = 20$ K close to $T_c$, the main source for the decay of the low-frequency phonons is due to the carrier–phonon interaction, while for the high-frequency phonons it is the defect and tunnelling state scattering. It is worth commenting that the main contribution to phonon scattering is from phonon–defect scattering at various temperatures as depicted in figures 2–5.

We first qualitatively discuss the properties of thermal conductivity due to phonons. Figure 6 shows our results for phonon thermal conductivity of YBa$_2$Cu$_3$O$_{7-\delta}$. As the temperature is lowered through $T_c$, the quasi-particle excitations condense into the ground state and they
cannot scatter phonons. The phononic thermal conductivity, thus, increases exponentially as the temperature decreases in the absence of other scattering mechanisms. Although the phonon thermal conductivity experiences an exponential increase below the transition temperature, the presence of the defects, the tunnelling states and the grain boundaries sets a limit on its growth; as a consequence, the phononic thermal conductivity diminishes as the temperature increases further.

The maximum position depends on the relative magnitudes of the phonon–carrier and phonon–defect interactions: below 5 K, the tunnelling states become the effective phonon scatterers and the thermal conductivity exhibits a typical $T^2$ behaviour; at even lower temperatures, grain-boundary scattering dominates and the usual Debye $T^3$ behaviour appears. Furthermore, $\kappa$ develops a broad peak at about one-half of $T_c$, before falling off at lower
Figure 5. Variation of various phonon relaxation times as a function of $x = \frac{\hbar \omega}{k_B T}$; $T = 100$ K.

Figure 6. Variation of phonon thermal conductivity as a function of temperature in the presence of various phonon scattering mechanisms.

temperatures; this is attributed to the fact that below $T_c$ the phonon mean free path increases with the decrease in temperature, as more and more carriers are condensed into the superconducting state. These are the features contained in equations (2) and (3) and are consistent with the earlier experimental observation [11].

We now turn to the calculation of the carrier thermal conductivity from equation (10). While estimating the electronic contribution we consider the standard physical parameters $\Delta(0) \approx 4.0$ meV, $T_c = 92$ K, $m^* = 5 m_e$, $Ze = -2e$ [15], $d = 3.2$ Å, $\epsilon_F = 0.25$ eV [26] and $\epsilon_c = 4.5$ [28] and we use the value of $N = 0.05$ [29] for YBa$_2$Cu$_3$O$_{7-\delta}$ superconductors. The analysis of elastic carrier–impurity contribution to the thermal conductivity is documented
Figure 7. Variation of normalized electronic thermal conductivity with reduced temperature \((T/T_c)\). In figure 7, it shows the variation of normalized carrier thermal conductivity of \(d_{x^2-y^2}\)-wave superconductors from equation (10) in \(\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}\). It is evident from the plot that \(\kappa_e\) decreases rapidly with the decrease in temperature and exhibits a power temperature characteristic in the whole temperature range.

We stress that \(\kappa_e\) increases with the increase in temperature and a rapid growth is reflected in the vicinity of \(T_c\) and is attributed to the condensed superconducting pairs at low temperatures. The other way round, i.e. in the low-temperature domain, the theoretical curve for normalized electronic thermal conductivity \(\kappa_e/\kappa_e(T_c)\) as shown in figure 7 shows that \(\kappa_e\) quasi-exponentially vanishes at low temperatures and becomes negligible below about 0.2 \(T_c\). Pairing symmetry of the order parameter in high-\(T_c\) cuprates is an important issue and is discussed with high intensity. The elastic scattering of carriers with impurities is important at low temperatures. The temperature dependence of the \(s\)-wave order parameter follows

\[
\Delta(T) = \chi k_B T_c \tanh \left[ \alpha \sqrt{\frac{T_c - T}{T}} \right].
\]

(14)

For an isotropic \(s\)-wave order parameter, the carrier–impurity thermal conductivity is a function of \(\exp(-\Delta(0)/k_B T)\). The elastic carrier–impurity contribution to thermal conductivity decreases below \(T_c\) and shows the signature of exponentially falling at low temperatures. On the other hand, the wavevector and temperature dependence of the \(d_{x^2-y^2}\)-wave order parameter is approximated by [3]

\[
\Delta(k, T) = \chi k_B T_c [\cos(\hat{k}_x) - \cos(\hat{k}_y)] \tanh \left[ \alpha \sqrt{\frac{T_c - T}{T}} \right].
\]

(15)

with \(\chi = \Delta(0)/k_B T_c\), where \(\Delta(0)\) is the zero-temperature gap parameter and \(\alpha \approx 2\). In the following, \(k_x = k_x a\) and \(k_y = k_y b\) with \(a\) and \(b\) the crystallographic parameters along the \(a\) and \(b\) axes, respectively. Hence, for an anisotropic \(d\)-wave order parameter, the carrier–impurity thermal conductivity shows a power law dependence. The elastic carrier–impurity scattering
Figure 8. Variation of normalized magnon thermal conductivity $\kappa_m(T)/\kappa_m(T_c)$ as a function of $T/T_c$.

contribution for the d-wave symmetry order parameter also decreases below $T_c$ but much less rapidly than in the case of the s-wave order parameter.

It is useful to address the role of vertex corrections at this point as we have not incorporated them while estimating the electronic thermal conductivity. For phonons with energies much smaller than the electron energy such corrections are small, as shown by Migdal [30]. Such a situation disappears when the boson energies become comparable to the Fermi energy. The assumption at the basis of the adiabatic Migdal–Eliashberg framework is Migdal’s theorem, which in principle states that, as long as the phonons have a much slower dynamics than that of the electrons, the non-adiabatic electron–phonon interference effects (vertex corrections) can be neglected. This condition is well satisfied in conventional superconductors since their Fermi energy is of order $\varepsilon_F \sim 10$ eV $\sim 10^5$ K, while the highest phonon frequencies are usually less than $\sim 50$ meV $\sim 600$ K.

However, in high-$T_c$ cuprates, the ratio of $\varepsilon_F/\omega_{ph}$ is about ten; the vertex corrections and other effects due to breakdown of Migdal’s theorem should have important consequences for the electron channel contributing to the thermal conductivity. In the present scheme, the contribution of the electron to the phonon thermal conductivity is about 0–1% in the temperature domain $0 < T < T_c$, and hence, if vertex corrections are important, our numerical results will not change significantly. For completeness, it is worth mentioning the work of Houssa and Ausloos [26], who argue that the vertex corrections will mix up electron–impurity–phonon contributions leading to nontrivial power-law dependence at finite temperatures. We now discuss the role of the spin-wave contribution to the thermal conductivity.

We plot the theoretical curve for the normalized magnon thermal conductivity $\kappa_m/\kappa_m(T_c)$ as shown in figure 8 for YBa$_2$Cu$_3$O$_{7-\delta}$ superconductors. For the actual calculation we need two free parameters and these are chosen as the effective magnon mean free path, $l_s$, of about 1.7 nm and the constant proportional to the exchange energy, $D \cong 0.83 \times 10^{-39}$ erg cm$^2$. It is worth mentioning that the spin correlation length in cuprates is larger than the lattice spacing $a$. It is noticed from equation (13) that $\kappa$ shows a power temperature dependence in the absence of an applied magnetic field (see the inset of figure 8). It is evident that $\kappa_m$ vanishes at low
temperatures and becomes negligible below about $0.1 \ T_c$. It is meaningful to comment that the contribution of the electrons and spin-waves to the phonon thermal conductivity is about 0–1% in the temperature domain $0 < T < T_c$. Phonons are, then, the sole carriers of heat in this temperature domain. On the other hand, in the low-temperature domain ($0 < T < 10$), magnon–phonon and electron–impurity contributions to the thermal conductivity are on the same footing at very low temperatures ($T \leq 4$ K), and at about 5 K the electron–impurity contribution diverges and increases sharply (see figure 9). The relative strengths of these two contributions lead to an increase in the thermal conductivity below $T_c$ and their contribution to the total thermal conductivity is marginal in comparison to the phonon thermal conductivity.

In principle, the thermal conductivity behaviour depends on the competition among the various scattering mechanisms for the heat carriers and balance between the electron, magnon and phonon competition. Finally, it is worth stressing that the maximum in $\kappa$ is around 60 K and is well reproduced from the present theoretical model (see figure 10). The peak at about 60 K is attributed to the shortened phonon mean free path as compared to that at low temperatures. Deduced results on temperature dependence of the thermal conductivity of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ from the present three-component model ($\kappa_e + \kappa_p + \kappa_{ph}$) are consistent with the experimental data [7]. We further comment that, despite this apparent consistency, the present scheme cannot accommodate the temperature independence of $\kappa$ above $T_c$, but shows a steep decrease.

We noted from the present calculations that $\kappa$ decreases in the normal state. Indeed above $T_c$ the temperature dependence of the phonon contribution is attributed to a competitive process in which $\kappa$ increases with increased temperature due to phonon–carrier scattering while $\kappa$ decreases with increased temperature due to phonon–phonon scattering. However, unlike conventional superconductors where the thermally excited quasi-particles of the electron system are dominant carriers of heat, in high-temperature superconductors the phonons are the dominant carriers of heat.

**Figure 9.** Relative contributions to thermal conductivity by phonons, electrons and magnons at low temperature.
4. Conclusions

The low-temperature thermal transport, i.e., thermal conductivity $\kappa$, behaviour is believed to be an instructive probe in understanding the role of phononic, electronic and spin excitations in cuprates. In order to simulate the actual situation occurring in the temperature dependent behaviour of thermal conductivity in high-$T_c$ cuprates, we consider three channels to $\kappa$, phonon, electron and magnon, within the relaxation time approximation. Developing this scheme, the present investigation deals with a quantitative description of temperature dependent behaviour of $\kappa$ in cuprates. The lattice thermal conductivity dominating in this cuprate is an artifact of strong phonon–defect and impurity scattering mechanisms below $T_c$. However, we have made a careful analysis taking into account several different processes that can exist in this cuprate whose interaction can yield the observed dependence. The fitting parameters in the present scheme that characterize the strengths of the phonon–defect, phonon–tunnelling state, phonon–electron and phonon–phonon scattering processes ($A = 4.9 \times 10^{-8} \text{ K}^{-3}$, $B = 1.47 \times 10^{-3}$, $P = 2.45 \times 10^{-3}$ and $C = 0.3 \text{ K}^{-6} \text{ s}^{-1}$) lead to a result that successfully retraces the experimental curve.

Generally, the interpretation of the experimental results is complicated because both carriers (either electrons or holes depending on the stoichiometry of the system) and the lattice contribute to the thermal conductivity and because both contributions are limited by various scattering mechanisms. Despite the limitations and use of free parameters for the estimation of coupling strengths, the present theoretical model of the thermal conductivity of the high-$T_c$ $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ superconductor consistently reveals the anomalous behaviour reported experimentally.

The present model calculations reveal that (a) in the low-temperature domain ($0.1 < T < 10\kappa$) documents an anomalous $T^2$ dependence on the temperature, (b) at temperature in the vicinity of $T_c$ $\kappa$ develops a broad peak, with a change of the slope, and (c) at and above $T_c$ a steep decrease. The holes as carriers in the present system that we have investigated...
are condensed into Cooper pairs, do not carry entropy and therefore cannot transport heat. Thus we expect a smaller contribution of carrier thermal conductivity below $T_c$. Also, the carriers that are bound into Cooper pairs can no longer scatter phonons. Precisely, the thermal conductivity behaviour in cuprates is strongly influenced by the competition among the various scattering mechanisms for the heat carriers and balance between the electron, magnon and phonon competition. Nevertheless, it has been found that the contribution of the electron and magnon channels towards thermal conductivity, when a comparison is made with the phonon thermal conductivity, is about 0–1% in the temperature domain $0 < T < T_c$.

However, if mainly carrier scattering limits the lattice thermal conductivity, one must expect an enhancement of lattice thermal conductivity below $T_c$. This is attributed to the fact that, below $T_c$, the phonon mean free path increases with the decrease in temperature, as more and more carriers are condensed into the superconducting state. Further, the origin of the peak at about 60 K is due to the shortened phonon mean free path as compared to that at low temperatures. In spite of this apparent consistency, the present scheme cannot accommodate the temperature independence of $\kappa$ above $T_c$, but shows a steep decrease. For good reasons discussed earlier, any operative superconducting mechanism on the high-$T_c$ YBa$_2$Cu$_3$O$_{7-\delta}$ superconductor must take into account the phonon–impurity and phonon–carrier couplings.

It is instructive to compare the thermal conductivity of Y–Ba–CuO superconductors with other high-$T_c$ superconductors. The overall size of the thermal conductivity in Y–Ba–CuO is larger than that of La–Sr–Cu–O, Ba–K–BiO, Bi–Sr–Ca–CuO (Bi-2212), Y–Ba–CuO (Y-124) and Tl–Ba–Ca–CuO (Tl-2223) systems. On the other hand, the magnitude of the thermal conductivity of electron-doped cuprates, such as Nd–Ce–CuO, is much larger than the hole-doped cuprates. Apart from this there is no anomaly reported in the vicinity of $T_c$ in electron-doped cuprates. We point out that the thermal conductivity in high-$T_c$ cuprates is much smaller than that of typical metals and comparable to that for amorphous materials.

In principle, below $T_c$, the charge carriers condensed into Cooper pairs carry no heat; the thermal conductivity is thus ensured by normal charge carriers. As the normal charge carrier scattering rate has been observed to decrease below $T_c$, thermal conductivity should increase in the superconducting state. The enhancement in the Y–Ba–CuO system is larger than La–Sr–CuO and is intimately related to larger $T_c$ as well larger phonon density of states. The difference of strengths of the enhancement in cuprates is also an important issue and needs detailed investigation of phonon scattering that is largely dominated by the lattice imperfections induced either by doping at parent site or by the oxygen deficiency. Depending upon the oxygen vacancies in the system, one can explore the relaxation absorption of phonons by the tunnelling process. However, one can only tentatively suggest the importance of oxygen vacancies in the formation of tunnelling states and hence in the thermal conductivity.

Analysis of transport measurements in the superconducting state of high-$T_c$ cuprate superconductors provides complete evidence of the pairing symmetry of the order parameter. With d-wave symmetry of the order parameter, we have estimated the carrier–impurity contribution for thermal conductivity and noticed that the elastic carrier–impurity scattering contribution for d-wave symmetry also decreases below $T_c$ but much less rapidly than in the case of s waves. At low temperatures, the behaviour of carrier thermal conductivity follows a power temperature law. Indeed, the theoretical results show that the reported thermal conductivity is comparable to the phonon thermal conductivity. More detailed information can be obtained from numerical evaluations of the transport coefficients of all high-$T_c$ cuprates. All this has to be covered in future studies.
The proposed model may, in spite of its simple structure, provide a consistent account for the experimental fact. We further comment that the treatment is incomplete. While estimating the electronic thermal conductivity, we have not incorporated the vertex corrections. However, in high-$T_c$ cuprates, the ratio of $\varepsilon_F/\omega_{ph}$ is about ten; the vertex corrections and other effects due to breakdown of Migdal’s theorem should have important consequences on the electron channel contributing to the thermal conductivity. In the present scheme, the contribution of the electronic channel to the phonon thermal conductivity is about 0–1% in the temperature domain $0 < T < T_c$, and hence, if vertex corrections are important, our numerical results will not change significantly. Hence, the behaviour of the thermal conductivity in cuprates is determined by competition among the several operating scattering mechanisms for the heat carriers and a balance between electron, magnon and phonon contributions.

Acknowledgment

Financial assistance from the Defence Research Development Organisation, New Delhi, India, is gratefully acknowledged.

References

[1] Bardeen J, Cooper L N and Schrieffer J R 1957 Phys. Rev. 106 162
[2] Ruvalds J 1996 Semicond. Sci. Technol. 9 905
  Kresin V Z, Wolf S A and Morawitz H 1993 Mechanisms of Conventional and High-$T_c$ Superconductivity (New York: Oxford University Press)
  Carbottle J P 1990 Rev. Mod. Phys. 62 1027
[3] Tsuei C C and Kirtley J R 2000 Rev. Mod. Phys. 72 969
  Scalapino D J 1995 Phys. Rep. 250 329
  Van Harlingen D J 1995 Rev. Mod. Phys. 67 515
[4] Varshney D, Patel G S and Singh R K 2003 Semicond. Sci. Technol. 15 1617
[5] Bardeen J, Rickayzen G and Tweordt L 1959 Phys. Rev. 113 982
[6] Morelli D T, Heremans J and Swets D E 1987 Phys. Rev. B 36 3917
[7] Uher C and Kaiser A B 1987 Phys. Rev. B 36 5680
[8] Nunez Regueiro M, Castello D, Izbizky M A, Esparza D and D’Ovidio C 1987 Phys. Rev. B 36 8813
  Tweel A, Tao Z C and Singh M 1991 Phys. Rev. B 43 11419
[9] Pintschovius L and Reichardt W 1998 Phonon dispersions and phonon density-of-states in copper-oxide superconductors Neutron Scattering in Layered Copper-Oxide Superconductors ed A Furrer (Dordrecht: Kluwer) pp 165–223
[10] Feile R 1989 Physica C 159 1
  Altendorf E, Chrzanowski J, Irwin J C and Franck J P 1991 Phys. Rev. B 43 2771
[11] Uher C 1992 Physical Properties of High Temperature Superconductors vol 3, ed D M Ginsberg (Singapore: World Scientific) p 159
[12] Nunez Regueiro M, Sales B, Calemczuk R, Marin C and Henry J Y 1991 Phys. Rev. B 44 9727
  Sera M, Shamoto S and Sato M 1990 Solid State Commun. 74 951
[13] Allen P B, Du X, Mihaly L and Forro L 1994 Phys. Rev. B 49 9073
  Houssa M and Ausloos M 1995 Phys. Rev. B 51 9372
[14] Mikhail I F I 1989 Phys. Rev. B 40 6828
[15] Houssa M, Bougrine H, Ausloos M, Grandjean I and Mehbod M 1994 J. Phys.: Condens. Matter 6 6305
[16] Hirschfeld P J and Putilka W O 1996 Phys. Rev. Lett. 77 3909

New Journal of Physics 5 (2003) 72.1–72.17 (http://www.njp.org/)
[17] Ausloos M and Houssa M 1999 *Semicond. Sci. Technol.* **12** R103
Varlamov A A and Ausloos M 1997 *Fluctuation Phenomena in High Temperature Superconductors (NATO ASI Partnership Subseries 3: High Technology)* vol 32, ed M Ausloos and A A Varlamov (Dordrecht: Kluwer) pp 3–41
Houssa M and Ausloos M 1996 *Proc. 10th Anniversary HTS Workshop on Physics Materials and Application* ed B Batlogg, C W Chu, D U Gubser and K A Muller (Singapore: World Scientific) p 328
[18] Bekeris V, Talpe J, Nunez Regueiro M, Malachevsky M T, D’Ovidio C and Serfaini D 1990 *Solid State Commun.* **75** 243
[19] Anderson P W, Halperin B I and Varma C M 1972 *Phil. Mag.* **25** 1
[20] Phillips W A 1972 *J. Low Temp. Phys.* **7** 351
[21] Golding B, Birge O, Haemmerle W, Cava R J and Rietman E A 1987 *Phys. Rev. B* **36** 5606
[22] Conardson S, Raistrick I and Bishop A R 1990 *Science* **248** 1394
Mustre de Leon J, Conardson S, Batistic I and Bishop A R 1990 *Phys. Rev. Lett.* **65** 1675
[23] Yu C C and Anderson P W 1984 *Phys. Rev. B* **29** 6165
[24] Callaway J 1991 *Quantum Theory of the Solid State* (London: Academic)
[25] Mahan G D 1981 *Many Particle Physics* (New York: Plenum)
[26] Houssa M and Ausloos M 1996 *Physica C* **265** 258
Houssa M and Ausloos M 1997 *Phys. Rev. B* **56** 953
[27] Douthett D and Friedberg S A 1961 *Phys. Rev.* **121** 1662
[28] Bozobic I 1990 *Phys. Rev. B* **42** 1969
[29] Houssa M, Feldmann J, Cloots R and Ausloos M 1998 *Semicond. Sci. Technol.* **11** 44
[30] Migdal A B 1958 *Zh. Eksp. Teor. Fiz.* **34** 404 (Engl. transl. 1958 *Sov. Phys.--JETP* **7** 996)
Eliashberg 1960 *Zh. Eksp. Teor. Fiz.* **38** 966 (Engl. transl. 1960 *Sov. Phys.--JETP* **11** 696)