Simulation analysis for the lattice thermal conductivity of YBCO superconductors

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The theory of Callaway for the lattice thermal conductivity, is extended to include the interference scattering between point defect and 3-phonon Umklapp-scattering (*U*-scattering). The experimental measurements of Ravindran and co-workers, in which radiation loss effects are minimized have been fitted by varying the parameters for boundary, sheet-like fault, point defect, 3-phonon scattering and the new scattering (interference scattering) terms. Since a large amount of disorder is present in YBCO samples, as emphasized by Kaiser, the interference scattering plays an important role in describing the phonon conductivity of these materials, particularly near the low temperature maximum. In the high temperature region ($T > 150$ K), where radiation losses become significant, the 3-phonon *U*-scattering term with exponential temperature dependence, leads to a good agreement with experimental data for the three different samples of YBCO superconductors.

THE lattice thermal conductivity measurements[1] on YBCO compounds have been extensively used to test the possible mechanism of superconductivity in these systems. An unexpectedly dramatic effect was discovered in the thermal conductivity of YBCO[1], viz. a strong increase below T_c. The same effect was independently discovered by several other groups[2–7]. These findings provide strong evidence that a large fraction of thermal resistivity above T_c arises from scattering of phonons by electrons; otherwise little change would be seen below T_c when the scattering disappears. Also, the scattering of phonons by electrons and by disorder is comparable (given relatively large amount of disorder in these materials). Assuming the electronic thermal conductivity remains small below T_c, would mean to find a mechanism whereby the phonon-system itself shows a dramatic change as the temperature drops below T_c. The electron–phonon coupling parameter as a function of temperature has been estimated and found reasonable[8], from a knowledge of variation in Debye temperature in the BCS (weak coupling) and Allen–Dynes (strong coupling) models for YBCO superconductors.

The phononic contribution to thermal conductivity is significant in the high temperature superconductors (HTS). The thermal conductivity of these solids, which promises wide applications for the future, has been reviewed by various workers[9,10]. The interpretation of thermal conductivity data for these materials becomes difficult due to the anisotropic nature of thermal conductivity, role of oxygen stoichiometry, dominance of phononic conductivity over the electronic counterpart, particularly below and near T_c, as the transition from metallic to superconducting phase is approached. The lack of knowledge about theoretical model for HTS and involvement of various other phonon scatterers such as magnons, also make the analysis difficult. Hence, the problem of analysing the thermal conductivity of HTS has recently been the subject of wide interest among various workers[11–14]. Ravindran *et al.*[11] have recently measured the T_c of YBCO pellets using plate-shaped samples, in the temperature range 7–260 K and have observed an opposite trend in the thermal conductivity curves above T_c, in contrast to the measurements of Uher and Kaiser[14] and Gottwick *et al.*[13]. In other earlier measurements made with rod-shaped samples, radiation losses were high and data above 150 K are not reliable using steady state axial flow heat conduction. This has encouraged us to investigate and analyse the thermal conductivity data of YBCO, as has been observed by Ravindran *et al.*[11], along with the measurements of earlier workers[12–14], using the model already proposed by us elsewhere[15]. The present analysis becomes rigorous and involves less approximations compared with other phenomenological models[16,17], which assume the validity of inverse summation rule for the relaxation time in the conductivity calculations.

In all the studies on samples of $YBa_2Cu_3O_7$ (YBCO) superconductors, the thermal conductivity starts increasing as sample is cooled below T_c. It reaches a maximum value around $T_c/2$ and decreases on further cooling. Using Wiedemann–Franz law, the electronic contribution to thermal conductivity is less than 10% of the total conductivity. Phonon contribution is dominant in this regard.

Kaiser[1], in order to probe the mechanism behind HTS, has analysed the thermal conductivity of YBCO. According to him, the observation of a peak in the thermal conductivity of YBCO leads fairly directly to an important conclusion. It provides strong evidence that a large fraction of thermal resistivity above T_c arises from the scattering of phonons by electrons, otherwise little change could be seen below T_c, when the scattering disappears. Also, that the scattering of phonons by electrons and by disorder is comparable is very surprising, given the relative large amount of disorder in these materials. It indicates a remarkably strong electron–phonon interaction. This has encouraged us to include the interference scattering term between defect and 3-phonon Umklapp-scattering (*U*-scattering), which is known to contribute dominantly near the low temperature maximum[15], in the present analysis of thermal conductivity for YBCO compounds. We also include the scattering due to sheet-like fault (present in the pellet samples) and the electron–phonon scattering and retain the exponential temperature-dependent 3-phonon scattering term in the analysis.

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In normal state, phonons are scattered by defect, electron and phonon. If the 3-phonon scattering be neglected, the defect and electron–phonon scattering lead to a slow increase in thermal conductivity with increase in temperature above T_c, in theoretical model of Tewordt and Wolkhausen[7]. Below T_c, charge carriers pair up to excitation spectrum. Phonons are not scattered by the condensate, but by the quasi-particle excitation which decreases rapidly in number as temperature is reduced below T_c. Consequently, the life time of phonon due to electron–phonon scattering increases as it contributes to thermal conductivity increase. On further cooling, the mean free path is limited by defect scattering and also thermal conductivity drops after passing through a maximum. The experimental measurements have been carried out by Ravindran *et al.*[11], using steady state flow heat conduction in plate-shaped samples, in order to minimize the radiation losses. Since the lateral surface area over which heat is conducted and radiation occurs is a fraction of the cross-sectional area, the error from radiation loss is enormously reduced in the measurements by Ravindran *et al.*[11].

They have measured the thermal conductivity of different samples of YBCO; pellet A with 78% density (sample A) and pellet B with 84% density (sample B) and have theoretically fitted their data for sample A, by including 3-phonon *U*-processes, in the Tewordt and Wolkhausen theory[7]. However, the fit is poor in the region $T \geq T_c$. In what follows, we analyse the different scattering mechanisms participating in heat transport, based on the modified Callaway model, to include the interference scattering and 3-phonon *U*-scattering in proper form, which may be important in HTS.

The expression for the lattice thermal conductivity can be written in the following form by introducing the reduced frequency $x = \beta\hbar\omega = (\hbar\omega/k_BT)$ and the reduced temperature $t\ (= T/T_c)$:

$$K = At^3 \int_0^\infty x^4 e^x/[(e^x - 1)^2 \cdot F(t, x)]\, dx, \qquad (1)$$

where the upper limit (Θ_D/T) has been replaced by ∞ and the function $F(t, x)$ representing the total relaxation rate (besides the common factor $A\ (= v/FL)$), is given by

$$F(t, x) = [1 + \alpha x^4 t^4 + \beta x^2 t^2 + \gamma t x g(x, y) + \delta x^3 t^4 + (\varepsilon_1 + \varepsilon_2 e^{-\Theta/aT}) x^2 t^5]. \qquad (2)$$

Here A, α, β, γ, δ, ε_1 and ε_2 refer to the scattering strengths due to the boundary scattering, point defect scattering, sheet-like fault, electron–phonon scattering, interference scattering (between point defect and 3-phonon processes) 3-phonon normal and *U*-scattering, respectively. Another term, $t\ (= T/T_c)$ is the reduced energy, where T_c is the transition temperature of $YBa_2Cu_3O_7$ superconductors. Also, $g(x, y)$ stands for the BRT function, defined by Bardeen *et al.*[18]. Equation (2) differs from that of Ravindran *et al.*[11] in the following way. In the first place Ravindran *et al.* have lumped the 3-phonon scattering coefficients ε_1 and ε_2 into a single coefficient ε and hence ignored the exponential dependence of *U*-processes contained in ε_2. Also, they have represented 3-phonon *U*-processes by the term $\varepsilon x^2 t^4$, which differs from that contained in eq. (2) above, that has been included by us in compliance with the variation considered earlier[15]. We have taken $a = 0.01$ in the present analysis.

Further, we have included the interference scattering term arising from the non-validity of the Methiessen's inverse summation rule, in our model. It is interesting to study whether any similar significant term (cross-term) arises between the other two scattering processes (such as between defects and *e–p* scattering processes, etc.) and whether they have any significant contribution in superconductors. This will be dealt with in future. Here we wish to examine the role of interference term in the thermal conductivity of superconductors, which has earlier been held responsible for conducting significantly near low temperature maximum in the semiconducting materials[15].

The experimental data for these different samples are taken from the measurements of Ravindran *et al.*[11] (squares–sample A, triangles–sample B) and Cohn *et al.*[12] (circles–sample C), as depicted in Figure 1. The result of theoretical fit based on eqs (1) and (2) is obtained separately for three different samples A, B and C considered by Ravindran *et al.*[11]. The values of different parameters used in the analysis are mentioned and corresponding responses are depicted. It is seen that the agreement between theory and experimental data for all different samples is satisfactory over the entire range of temperature.

We have analysed the thermal conductivity of YBCO for three samples. The following analysis has been carried

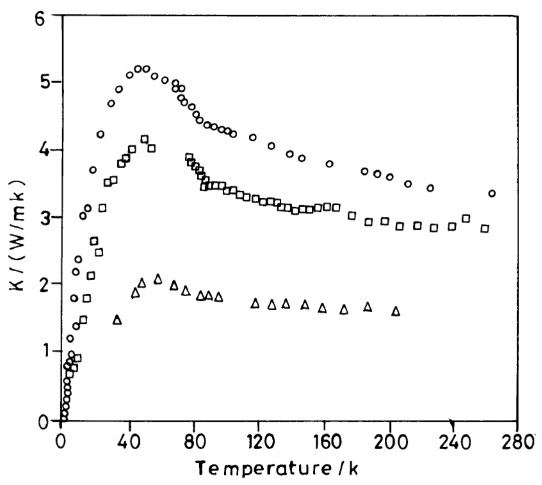

Figure 1. K vs T graph of YBCO samples: □, sample A; Δ, sample B; O, sample C (Cohn *et al.*[12]).

out so as to get the consistency with the experimental data for all three samples.

In analysing sample A, the best fitted values for two sets of parameters have been obtained in the temperature range of 10 to 260 K. This has been shown by the continuous curve plotted in the Figure 2 along with the theoretical fit (dashed line) of Ravindran *et al.*[11]. The values of different parameters used by us and other workers for thermal conductivity analysis are given in Table 1.

Similarly, for sample C, the best response with the experimental results is shown in the curve plotted in the Figure 3. The values of various parameters obtained are shown in Table 2. Thus the agreement with observations of Cohn *et al.*[12] seems reasonable, as evident from Figure 3.

The response shown in Table 2 for sample B is found best fitted with the experimental data and has been plotted in Figure 3 for sample B. The agreement with observations of Ravindran *et al.*[11] for this sample, is reasonably good over the entire range of temperature.

In the present work, we have analysed the thermal conductivity of three different samples of YBCO compounds, in the range 7–260 K, based on the measurements of Ravindran *et al.*[11] and Cohn *et al.*[12]. The analysis is based on a modified Callaway model that does not explicitly assume the validity of inverse summation rule for the relaxation time, which in fact, holds only as an approximation. These considerations lead to a cross (or interference) term of defect (mass-defect) with the 3-phonon *U*-scattering in the total relaxation rate that appears in the analysis of lattice thermal conductivity in these systems. This is also supported by the fact that a large amount of disorder is also present in these materials. The inclusion of interference scattering along with boundary scattering, point defect scattering, electron–phonon scattering and scattering due to sheet-like faults (present in the pellet samples) in the present modified model for the lattice thermal conductivity, yields fairly good results for the three samples of YBCO compounds.

In the present analysis, the thermal conductivity increases gradually below T_c (approached from above), as seen by the continuously rising curve instead of an abrupt increase, pointed out for sample A by Ravindran *et al.*[11] (Figure 2). However, a good agreement is achieved between the present theory and experimental data for sample B, based on the measurements of Ravindran *et al.* The measurements on rod-shaped samples (sample C) have also been achieved by the present theory, over the entire range of temperature (Figure 3). For sample A, we have also used another set (ii) of parameters (Table 1) ignoring the exponential temperature dependence of the 3-phonon *U*-scattering term (which now varies as $\varepsilon x^2 t^5$, both ε_1 and ε_2 being lumped into one parameter ε), which leads us closer to the measured values near T_c but deviates considerably above 150 K when the radiation losses become significant, as revealed by Ravindran *et al.*[11]. Therefore, above 150 K, when the radiation loss become significant, the 3-phonon scattering, should be included with proper temperature dependence (exponential) of the

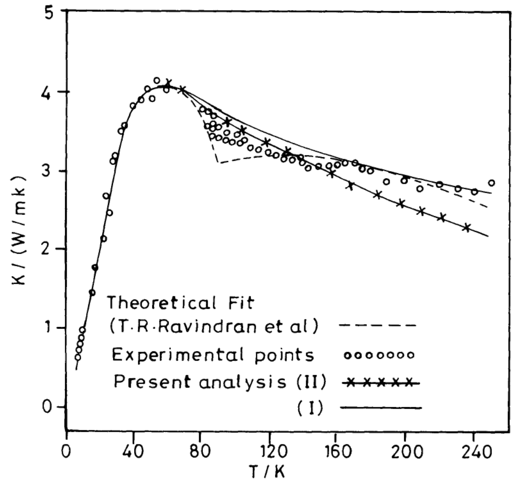

Figure 2. *K* vs *T* graph of YBCO samples.

Table 1. Comparison of parameters used to achieve consistency

Reference		A	γ	α	β	ε	ε_1	ε_2	δ
Uher and Kaiser[14]		3.5	100	50	60	0	–	–	–
Gottwick *et al.*[13]		5.0	100	60	35	0	–	–	–
Ravindran *et al.*[11]		2.0	50	20	35	30	–	–	–
Present study	(i)	4.0	50	15	50	–	0.02	0.01	200
	(ii)	4.0	25	10	60	0.2			200

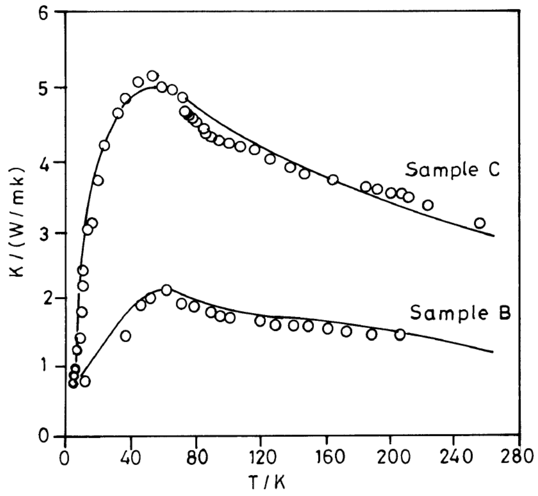

Figure 3. *K* vs *T* graph of YBCO samples.

Table 2. Thermal conductivity for sample C and sample B

Sample	A	γ	α	β	ε_1	ε_2	δ
C	4.8	300	60	35	0.02	0.02	150
B	1.05	100	20	18	0.02	0.02	150

U-scattering term. This leads us to a better fit above 200 K, as seen for sample A (Figure 2), where the fit of Ravindran *et al.*[11] falls below the experimental points. This fact is also evidenced by the fitness achieved for other two samples in the region $T \geq 150$ K. The fit for sample A near T_c can be further improved by increasing the value of γ (the electron–phonon scattering coefficient responsible for opening the gap near T_c) with respect to δ, and varying the parameter a.

It is concluded from the present work that the proper inclusion of exponential temperature dependence in the 3-phonon U-scattering processes, leads to good consistency in the thermal conductivity curve beyond 150 K, where the radiation losses become significant. In contrast, the fit of Ravindran *et al.*[11], who exclude the above exponential term in their calculations, falls much below the experimental data beyond 200 K. Also, in the vicinity of low temperature maximum (around 45 K), it is the interference scattering between point defect and 3-phonon processes, that contributes significantly to achieve consistency with the experimental results. This term is important in these materials as relatively large amount of disorder is present.

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Hottest April of the 20th century over north-west and central India

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The year 1999 witnessed unprecedented heat in the month of April in which most parts of north-west and central India recorded maximum temperatures of 40°C or above for about a fortnight, which is a record event of the 20th century. Increase in maximum temperature started right from the beginning of the month and conditions became extreme during the last week. Temperature records of the previous years indicated warm Aprils in the years 1892, 1921, 1931, 1941, 1958, 1973, 1980 and 1988 but not on the scale at which heat-wave conditions were experienced in 1999 over north-west and central India. This is seen in terms of mean maximum temperatures at 28 stations in that region. The study shows that about 72% of these stations recorded mean maximum temperature above 40°C. The occurrence and persistence of this hot spell in April 1999 appears to be a unique feature of the 20th century.

Raghavan[1] has examined departure of maximum temperatures from normal in April for the period 1911 to 1961 and Bedekar *et al.*[2] discussed details of the synoptic systems which favour the severe heat wave over India on a broad scale. De and Mukhopadhyay[3] have studied the severe heat wave conditions in the country which prevailed in May 1998, in perspective of global climate. Desai *et al.*[4] have studied the heat wave days for the months of March to June for the period 1990–1995 and concluded that drought/good monsoon years have no relation with number of heat wave days. All these studies indicate that frequency and intensity of heat waves are maximum in May and June over India and they are less frequent in April. Emphasis in these studies is on the individual heat wave epochs and their frequencies. This does not indicate whether a particular April as a whole has been anomalously warm or not. Climatology of mean maximum temperatures of April has not been addressed in any of these studies. Data series of mean maximum temperatures of New Delhi and a few other stations in the north-west and central India indicate peaks in some years like 1892, 1921, 1931, 1941, 1958, 1973, 1988 and 1999. Taking these as anomalously warm years, the mean maximum temperatures for all these years were computed in respect of 28 stations in the north-west and central India, where highly pronounced heat wave conditions occurred in 1999. Some of the climatological features of April's

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