

Anisotropy in Heat Conduction in Layered Cuprate HTS Hg-1212

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Abstract

$\text{HgBa}_2\text{CaCu}_2\text{O}_{6+\delta}$ (Hg-1212), the two- CuO_2 -layer member of the mercury-cuprate family $\text{HgBa}_2\text{Ca}_{n-1}\text{Cu}_n\text{O}_{2n+2+\delta}$, has been one of the most intensively studied cuprate high-temperature superconductors since its discovery in 1993. With an exceptional critical temperature (T_c) is about 120–150 K, a nearly flat CuO_2 plane, and an uncomplicated tetragonal structure, Hg-1212 can be harness as both a technologically promising HTS and a model system to investigate the onset of superconductivity in cuprates. The present work explores the various scattering phenomenon and thermal conductivity in the frame work of in-plane and cross-plane scenario by employing quantum dynamical method. This will employable as a tool for better understanding of mechanism and importance of CuO_2 planes in cuprate high temperature superconductors.

Keywords: Anisotropy, Heat Conduction, Quantum Dynamical Method

1. Introduction

The discovery of superconductivity in the $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ system by Bednorz and Müller in 1986 [1] triggered a search for cuprate compounds with ever higher transition temperatures of about 30-35 K. In the successive year 1987, another cuprate high temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ was discovered by Maw-Kuen Wu and Paul C.W. Chu [2] with transition temperature greater than boiling point of liquid nitrogen. Within the family of layered high temperature superconductors, the Bismuth, Thallium or Mercury-based cuprate HTS emerged relatively late but proved exceptionally rewarding. Putlin *et al.* [3] reported superconductivity at 94-98 K in the single-layer compound $\text{HgBa}_2\text{CuO}_{4+\delta}$ (Hg-1201) in 1993, and then Schilling and co-worker reported superconductivity above 130 K in the two-layer $\text{HgBa}_2\text{CaCu}_2\text{O}_{6+\delta}$ (Hg-1212) and three-layer $\text{HgBa}_2\text{Ca}_2\text{Cu}_3\text{O}_{8+\delta}$ (Hg-1223) phases. Latterly, Chu and coworkers [4,5,6] subsequently showed that the transition temperature of Hg-1223, pushes the above 150 K under hydrostatic pressure of about 30–45 GPa—the highest confirmed T_c of any material for more than two decades.

Within this series, Hg-1212 [6] occupies an important middle position. The number of CuO_2 layers per unit cell is lower than that of the three CuO_2 layered Hg-1223 but higher than the single layered Hg-1201. Also, it is consistent with the general trend in multilayer cuprates high temperature superconductors (HTS) that T_c initially rises with the number of CuO_2 layers per unit cell before declining again beyond three layers. Among the family of Hg-based cuprate HTS, the Hg-1212 is comparatively simple, with a high T_c at ambient pressure, and can be utilize as an important test bed for structure–property relationships across the whole cuprate family.

In the present work, we compare the structural properties of Hg-1212 with YBCO. Also, the anisotropic behavior of heat transport in Hg-1212, that is the in-plane thermal conductivity is larger than the cross-plane thermal conductivity by employing the quantum dynamical technique.

2. The HTS Hg-1212

High-temperature cuprate superconductors $\text{HgBa}_2\text{CaCu}_2\text{O}_{6+\delta}$ (Hg-1212) have a layered perovskite-like structure of ABX_3 type, in which "X" is a negatively charged anion (often oxygen or halogen) and "A" and "B" are positively charged cations. In Hg-1212, the "1212" represents the one -Hg layer, two -Ba layer, one -Ca layer, two -Cu layers.

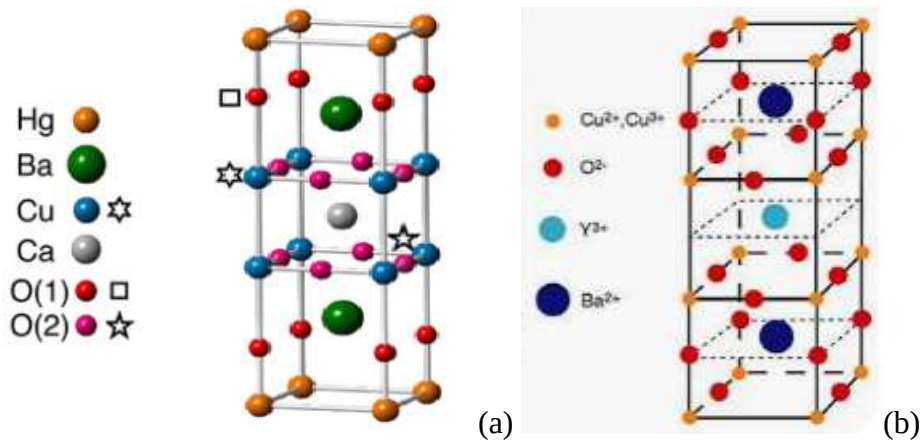


Fig. 1: Unit cell of (a) Hg-1212 [7] (b) $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ [8]

The structure of YBCO is orthorhombic ($a \neq b \neq c$ with $a=3.82$, $b=3.89$, $c=11.68$) in nature whereas Hg-1212 is tetragonal ($a=b \neq c$ with $a=3.85$, $b=3.85$, $c=12.65$) in nature and they are quite similar in structure with Ca replacing the chains -CuO- [9]. Both has two CuO_2 planes per unit cell. All layered cuprates HTS contains successive conduction layers and binding layer, the binding layer sometime known as charge reservoir layer. Conduction layers contain copper-oxide (CuO_2) planes of the type shown in above figure with each copper ion (Cu^{2+}) is surrounded by four oxygen ions (O^{2-}). As shown in Fig. 1(a), CuO_2 planes are bound together in the structure by a binding layer that contains calcium (Ca^{2+}) ions. In contrast, the intervening ions in the YBCO molecule are yttrium (Y^{3+}) rather than calcium. In the superconducting state below T_c , the formation of pairon take place via mediated phonon, that carry the supercurrent in the planes. In the normal state above T_c the conduction electrons released by copper atoms move about on these CuO_2 planes carrying electric current. The heat conduction in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ is highly anisotropic in nature, that is the heat transport along the CuO_2 plane (in-plane) is larger than cross-plane [10], referring to this the heat conduction in Hg-1212 has been evaluated and found similar behavior in thermal conductivity curve.

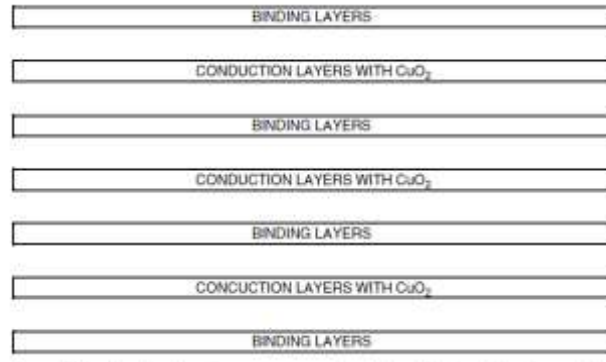


Fig. 2: Layering scheme of a cuprate superconductor [7].

3. Anisotropy in Heat Transport in Hg-1212

For studying structural anisotropy, the in-plane and cross-plane thermal conductivity of Hg-1212 has been evaluated. As stated earlier, the cuprate HTS are well known for their anisotropic behavior and layered structures, namely; conduction layer (CuO₂), charge reservoir or binding layer (MO), (where M is a metal atom), which allow one to study the thermal conductivity in the anisotropic scenario. In the previous work[10] the in-plane and cross-plane thermal conductivity for YBCO has been explored, then compared with the experimental work of Hagen *et al.* [11] and found excellent results. We note that for YBCO, the magnitude of in-plane thermal conductivity ($\kappa_{\parallel}$) is much larger than the cross-plane ($\kappa_{\perp}$). This indicates (i) a strong scattering of the phonons due to the weak inter layer bonding of ions along the 'c' direction, and (ii) a weak scattering due to strong in-plane bonding (fig. 3) [10]. Also, a granular sample (or polycrystalline/nanocrystalline material) typically has lower thermal conductivity than a single crystal of the same material [12]. The superconductor Hg-1212 has similar structure as YBCO, referring to that, the in-plane and cross-plane thermal conductivity has been evaluated for Hg-1212 by employing quantum dynamical method.

Present theory has been so evolved that there are no adequacies involved in the Callaway model, like absence of appropriate dispersion of phonons and incorrect use of relaxation times τ_i , violating Matthiessen's rule [13,14] and was taken up in the form of line width. Therefore, the thermal conductivity has been evaluated using modified Callaway's model in the in-plane and cross-plane scenario [10,17]:

$$\kappa = \sum_i \left(\frac{k_B}{2\pi^2 v} \right) (\beta^2 \hbar^2) \int_0^{\omega_D} \tau_i \frac{\omega_i^4 e^{\beta \hbar \omega_i}}{(e^{\beta \hbar \omega_i} - 1)^2} d\omega_i; \quad i \equiv ab, c \quad (1)$$

$$\tau_k^{-1}(\omega) \approx \tau_{CB}^{-1}(\omega) + \Gamma_k^D(\omega) + \Gamma_k^{3A}(\omega) + \Gamma_k^{AD}(\omega) + \Gamma_k^{ep}(\omega) + \tau_R^{-1}(\omega) \quad (2)$$

where the superscripts D, 3A, AD and ep refers to the contributions coming from defect scattering, anharmonic phonon-phonon scattering, impurity-anharmonicity interference scattering and electron-phonon scattering, $\tau_{CB}^{-1}(\omega)$ and $\tau_R^{-1}(\omega)$ are the combined boundary and resonance scattering relaxation times, respectively. The role of various scattering processes for in-plane and cross-plane has also been explored in next section.

4. The Role of Various Scattering

This section reveals the behaviour of inverse relaxation times (or line-width) that depends on impurity or

defects concentration, phonon-phonon interaction, interference modes etc. terms very distinctively for in-plane and cross-plane. The HTS Hg-1212 cuprates consist of tetragonal CuO_2 planes (the ab-plane) stacked on top of each other along the c-axis, thus forming layered structure as shown in Figure-1(a). The detail definition and terms involved in various scattering phenomenon are defined elsewhere [8] and no need to replicate here.

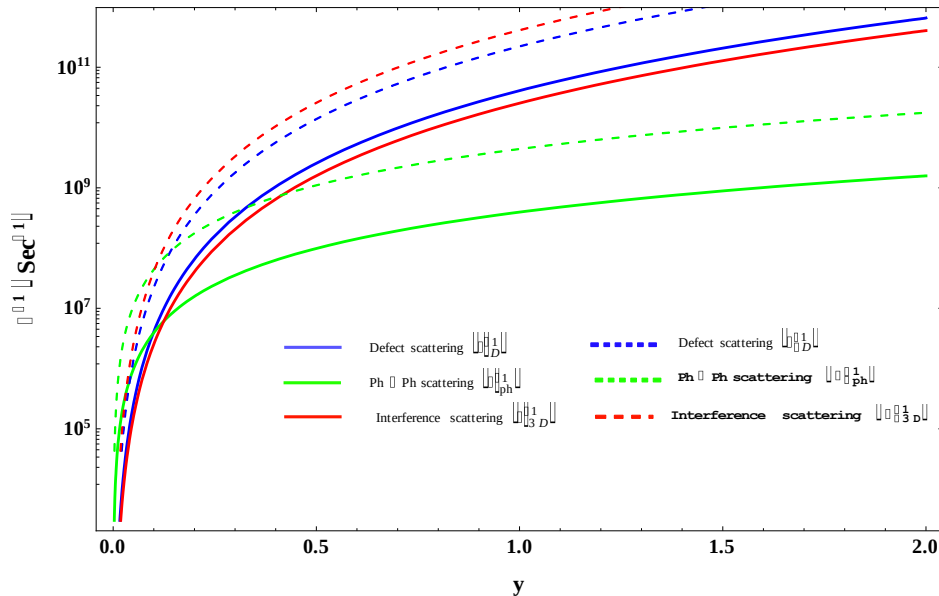


Fig. 3: The variation of inverse relaxation time for different scattering with reduced frequency ($y = \hbar\omega/k_B T$).

The above figure shows the variation of inverse relaxation time (or line-width) for different scattering with reduced frequency ($y = \hbar\omega/k_B T$) at fixed temperature around T_c . The thick blue, green and red line represents the defect, phonon-phonon and inference scattering, respectively, for ab-plane while the dashed blue, green and red line showing the same scattering along c-axis. It is clearly seen in above figure that the cross-plane scattering (weak inter-layer bonding) is much more pronounced than in-plane scattering, (strong in-plane bonding) resulting the larger in-plane conductivity in contrast to cross-plane conductivity (figure 4). Also, the defect scattering is largest among all three scattering.

5. Results and Discussions

The values of the various coefficients used in calculating the in-plane and cross-plane thermal conductivity of Hg-1212 have been listed in Table 1. It is evident that the values of the two types of coefficients (in-plane and cross-plane) exhibit anisotropy. The weak interlayer bonding in these layered HTS resulting in stronger scattering in the cross-plane direction, leading to smaller thermal conductivity ($\kappa_{\perp}$). The plot (Fig.-3) for inverse relaxation time (line-width) vs reduced frequency for different scattering phenomenon (defect scattering, multi-phonon scattering and the interference scattering) is also validate this anisotropic behavior of Hg-1212

In particular, defect scattering, multi-phonon scattering, and interference scattering exhibit anisotropy. Thus, one may conclude that the heat transport in Hg-1212 inherits the anisotropy primarily due to these scattering processes, that depends on the direction of the heat conduction. Therefore, $\kappa_{\perp}$ is much smaller than the $\kappa_{\parallel}$. The comparatively significantly smaller size of $\kappa_{\perp}$ indicates that these materials have weak

cross-plane heat conductivity. Thus, this highly anisotropic material can be employable for such applications where the material is required to thermally conduct efficiently only in a direction. It is obvious from Figure-4 that the in-plane thermal conductivity dominates over cross-plane thermal conductivity over whole of the temperature range in the superconducting regime.

TABLE 1. Constants and parameters used in the analysis of thermal conductivity of $\text{La}_{2-x}\text{S}_x\text{CuO}_4$

Hg-1212	B(I) ($\times 10^{-2}$)	A ($\times 10^{-43}\text{s}^3$)	B ($\times 10^{-21}\text{s K}^{-1}$)	D ($\times 10^{-44}\text{s}^3\text{K}^{-1}$)	A1 ($\times 10^2\text{erg}^{-2}\text{K}^{-2}$)	A2 ($\times 10^2\text{erg}^{-2}\text{K}^{-2}$)	R ($\times 10^{30}\text{s}^3$)
ab-plane	1.11	1.740	6.830	1.135	8.58	8.58	1.041
c-axis	1.21	14.87	75.98	18.44	8.78	8.78	0.527

Thus, the CuO_2 planes, which are responsible for pairon formation [Charles poole] and thus onset of superconductivity, is also the entity for the main thermal transport. Further, as indicated in Figure-4, the cross-plane thermal conductivity nearly saturates at fairly low temperatures, after which it becomes almost temperature insensitive. This property can be harness and may be employed as fabrication of such devices where constancy of thermal transport in desirable direction for particular temperature range of interest. The in-plane thermal conductivity exhibits strong temperature dependency and going to decline near transition temperature (T_c) as the heat carriers (electron or phonon) may involve in pairon formation.

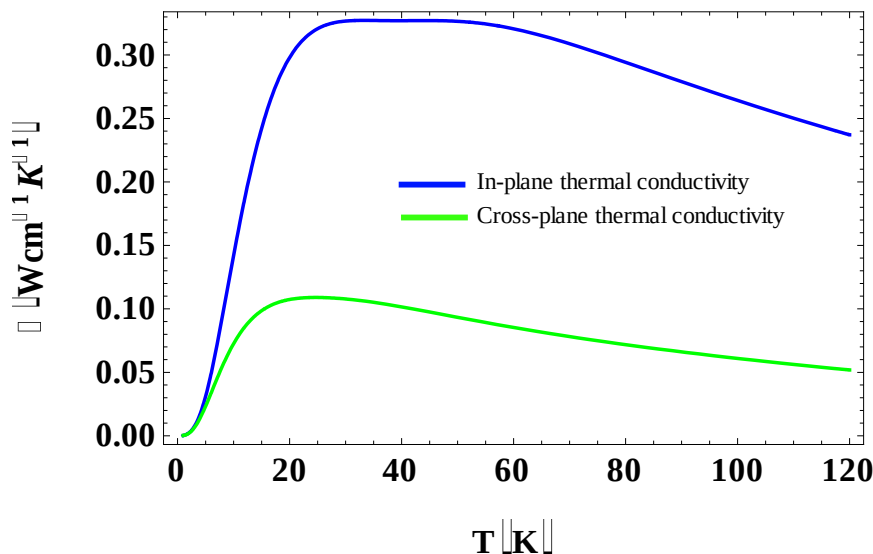


Fig. 4: In-plane and cross-plane thermal conductivity of Hg-1212

6. Conclusions

It emerges from present study that the thermal transport in Hg-1212 can successfully explain the anisotropic behavior of thermal conductivity and is applicable to all layered cuprate HTS. Additionally, the present investigation support that the thermal conductivity parallel to the CuO_2 layers is consistently greater than that perpendicular to the layers. Also, the scattering is more prominent along the cross-plane resulting less conduction across the plane. This concept can be used technologically to fabricate devices that are cool in the cross-plane direction yet heated in the in-plane direction.

7. References

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