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Thermal Diffussivity In Mercury Doped Superconductors

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***Abstract*—We analyse the effect of thermal diffusivity on the critical temperature of mercury-doped superconductors by employing theoretical technics. Thermal diffusivity, γ gives the rate at which heat is propagated through the material medium during changes in temperature with respect to time. Thermal conductivity gives useful information on the structure of the superconducting energy gap in Cuprates. In this work, thermal diffussivity is derived from thermal conductivity by considering both electronic and phononic contributions to heat currents in the superconductor. It is observed that for high critical temperatures to be achieved thermal diffusivity on the surface of the superconductor should be as high as possible. High oxygen doping level reduce thermal diffusivity and hence lowers the ability of the superconductor to a achieve the highest Tc. Room temperature superconductivity is possible in Hg1201 if the diffusivity is 68m^3/s and in Hg1223 if diffusivity is 26m^3/s.**

Keywords—Thermal Diffussivity, thermal conductivity, specific heat, transition temperature

1. INTRODUCTION

Cuprate superconducting materials have CuO_2 plane which acts as charge reservoirs. They are slightly doped by holes or electrons as charge carriers whose concentration differs from one Cuprate to another to make them superconductors. Cuprates super conduct at temperatures above 30k, therefore they are classified as high-T_C superconductors. Thermal fluctuations are much more important in the high-T_C Copper oxide superconductors due to rise in thermal energy in their superconducting state. The most striking effects of enhanced thermal fluctuations in the high-T_C superconductors are found in an applied magnetic field. The t-J-d model of high-Tc superconductivity (Rapando, *et al*., 2015), predicts heat capacity of $YBa_2Cu_3O_7$ at the critical temperature as 4.7×10^{-3}eVK^{-1} meaning that the superconducting transition is a function of thermal energy. In our work, we set out to determine the effect of diffusion of this thermal energy on critical temperature of mercury doped superconductors.

Experimental observations using YBCO (Uher, *et al.,* 1994), reveals that thermal conductivity exhibits a dramatic increase below T_C which results in a pronounced peak near $T_C/2$. A sharp decrease in the quasiparticles scattering rate below T_C is revealed. The peaks arise from the enhancement in the mean free path of phonons as the charge carriers undergo condensation since there is clear indication that quasiparticle transport is highly unusual.

Thermal conductivity in $YBa_2Cu_3O_{7-\delta}$ decreases with increasing magnetic field (Mbalaha, *et al*., 2011). This anisotropic behaviour of thermal Conductivity is due to increase in scattering rate of electrons by the collision of the Core of the vortices. There is saturation of the thermal conductivity at higher fields as a result of increase in normal electron density to compensate the scattering rates of electrons. The superconducting energy gap decreases with increasing magnetic field and temperature in the superconducting state. The energy gap is overcome when the temperature in the superconductor exceeds its critical temperature.

Measurements of heat transport in the Cuprate superconductors $YBa_2Cu_3O_y$ and $La_{2-x}Sr_xCuO_4$ at low temperatures as a function of doping reveals a residual linear term κ/T throughout the superconducting region and it decreases steadily as the Mott insulator is approached from the over doped region (Keimer, *et al.,* 2015). The low-energy quasiparticle gap extracted from κ/T is seen to scale closely with the pseudo gap. The presence of nodes and the tracking of the pseudo gap show that the overall gap remains of the pure d-wave form throughout the phase diagram, which excludes the possibility of a complex component appearing at a putative quantum phase transition and argues against a non-superconducting origin to the pseudo gap.

The presence of fluxoids in the mixed state of high-T_C superconductors alters the heat transport (Kralik, *et al*., 2017). The fluxoid structure serves as an additional scattering Centre for the phonons at temperatures below T_C where phonons dominate the heat transport and electronic excitations typically near T_C where the electronic excitations are plentiful, this promotes the heat transport in the superconducting state of high-T_C superconductors. The heat transport in the presence of a domain wall is inherently anisotropic and non-local. The bound states in the non-uniform region in the superconductor plays a crucial role in controlling heat transport since they modify the spectrum of quasiparticle state and hybridize the impurity band to produce a local transport environment, (Richard, C. and Vorontsov, B. A., 2016). As a result of this interplay, heat transport becomes highly sensitive to temperature, magnetic fields and disorders. Therefore its effect to critical temperature cannot be underestimated. Our research has considered the heat transport at the critical temperatures of high-T_C mercury doped cuprate superconductors and its effect on the transition temperatures of these superconductors.

2. THEORETICAL CALCULATIONS

The electronic heat carriers in the superconducting state are unpaired electrons whose concentration is n_e. Thermal conductivity in superconductors is necessitated by these electrons which are scattered by the core of vortices in the mixed state. The scattering rate of the Electronic heat carriers due to excitations in the core of vortices (τ_{e-v}^{-1}) is given by (Mbalaha, *et al,* .2011);

$$\tau_{e-v}^{-1}=\alpha\,(T)\frac{B}{\mu_0 H_C} \quad \text{……………1.1}$$

Where, B is the magnetic flux, μ_0 is the permeability in the free space, H_C is the upper critical magnetic fields and α(T) is the scattering constant which varies with temperature and is given as;

$$\alpha\,(T)=\frac{e^5\mu_0 H_C}{C\hbar^2 E_F^2}\sum_J \frac{\sqrt{\Delta_{(0)}^2-\varepsilon_J^2}}{1+\exp(\frac{2\varepsilon_J}{K_B T})} \text{.....1.2}$$

Where c is the velocity of light in free space, E_F is the Fermi energy, ε_J is the energy of a quantum state , K_B is the Boltzmann constant and Δ_0 is the energy gap in the limit of T→0.

The upper critical magnetic field H_C in the superconducting state can vary with the coherence length ξ, as, (Andrei, 2004).

$$H_C=\frac{\emptyset_0}{2\pi\mu_0\xi^2} \text{ ....1.3}$$

Where, $\emptyset_0$ is the magnetic flux contained in a fluxoid.

Substituting equation 1.3 into 1.2 to obtain;

$$\alpha(T)= \frac{e^5\emptyset_0}{2\pi C\hbar^2 E_F^2\xi^2}\sum_J \frac{\sqrt{\Delta_{(0)}^2-\varepsilon_J^2}}{1+\exp(\frac{2\varepsilon_J}{k_B T})} \text{ ...1.4}$$

The magnetic field relates with temperature T, in the superconducting state as, (Nie and Williams, 2016).

$$H_C(T)=H_0\{1-(\frac{T}{T_C})^2\} \text{..................1.5}$$

Where, H_0 is the upper critical field at absolute zero temperature.

To obtain the relation between the scattering rate of electronic heat carriers and temperature in the superconducting state equation 1.4 and 1.5 is substituted into 1.1 to give;

$$\tau_{e-v}^{-1}=\frac{e^5\emptyset_0 B}{2\pi\mu_0 C\hbar^2 E_F^2\xi^2 H_0\{1-(\frac{T}{T_C})^2\}}$$

$$\sum_J \frac{\sqrt{\Delta_{(0)}^2-\varepsilon_J^2}}{1+\exp(\frac{2\varepsilon_J}{k_B T})} \text{.....................1.6}$$

Equation 1.6 shows how the rate of scattering of electronic heat carriers due to excitation in the core of vortices varies with the temperature in the superconducting state.

2.1 Total Thermal conductivity in the superconducting state.

The current decays exponentially as it penetrates into the interior of a superconductor, it is essentially a surface current. The Meissner effect is accompanied by a surface current and it is this current which acts to shield the inner superconductor from the external magnetic field resulting in a perfectly diamagnetic medium, the magnetic field due to the surface current completely cancels the external magnetic field in the medium. This current is obtained by London's 2nd equation, (Andrei, 2004), which is given by;

$$J_z = -\left(\frac{n_c e^2}{\mu_0 m}\right)^{\frac{1}{2}} B_y(0)\exp^{-\frac{x}{\lambda_L}} \text{ ...1.7}$$

Where, J_z is the superconducting current density, λ_L is the London's penetration depth, m is electron effective mass, $B_y(0)$ is the magnetic flux on the surface of the superconductor, x is the thickness of the superconductor and n_c is the concentration of superconducting electrons.

To determine the concentration of superconducting electrons, n_c , equation 1.7 is re-arranged as,

$$n_c = -\frac{\mu_0 m J_z^2 exp\frac{2X}{\lambda_L}}{B_y^2(0)e^2} \text{ ....1.8}$$

The total Electronic contribution to thermal conductivity is given by; (Mbalaha, *et al*,.2011).

$$k_{elec}=k(T,0)+k_{e-v}(T,B) \text{ ....1.9}$$

Here, k (T,0) is the thermal conductivity in the absence of magnetic field, given by;

$$k\,(T,0)=\frac{1}{3m}n_e\pi^2 K_B^2 T\tau \text{ ....1.10}$$

Where, n_e is the normal electron concentration and τ is electron relaxation time.

$k_{e-v}\,(T,B)$ is thermal conductivity due to scattering of electrons by the vortex cores which is given by;

$$k_{e-v}=\frac{\pi^2}{3}\frac{k_B^2 T}{m}n_c\tau_{e-v} \text{ ....1.11}$$

Substituting equation 1.8 into 1.11 gives;

$$k_{e\text{-}v}=-\frac{\pi^2}{3}\frac{k_B^2 T}{m}\frac{\mu_0 m J_z^2 exp\frac{2X}{\lambda_L}}{B_y^2(0)e^2}\tau_{e-v} \quad .....1.12$$

Scattering rate of electronic heat carriers due to the excitation in the core of vortices depends on the applied magnetic field and it is given by equation 1.6, Substituting its reciprocal to 1.12 gives the thermal conductivity in a magnetic field caused by the scattering of electrons in the vortex cores.

$$k_{e\text{-}v} = -\left(\frac{\pi^2}{3}\frac{k_B^2 T}{m}\right)\left(\frac{2\pi\mu_0 C\hbar^2 E_F^2\xi^2 H0\left\{1-(\frac{T}{T_c})^2\right\}}{e^5\emptyset_0 B}\right)\left(\frac{\mu_0 m J_z^2 exp\frac{2X}{\lambda_L}}{B_y^2(0)e^2}\right)\sum_J \frac{1+\exp(\frac{2\varepsilon_J}{k_B T})}{\sqrt{\Delta_{(0)}^2-\varepsilon_J^2}} \quad ....1.13$$

Simplifying equation 1.13 gives,

$$k_{ev}=-\frac{2}{3}\left(\frac{\pi^3\mu_0^2 k_B^2 T C\hbar^2 E_F^2\xi^2 H0\left\{1-(\frac{T}{T_c})^2\right\}J_z^2 exp\frac{2x}{\lambda_L}}{\emptyset_0 B e^7 B_y^2(0)}\right)\sum_J \frac{1+\exp(\frac{2\varepsilon_J}{k_B T})}{\sqrt{\Delta_{(0)}^2-\varepsilon_J^2}} \quad ....1.14$$

Equation 1.14 gives Magneto-thermal conductivity as a result of Meissner effect where the surface current shields the inner Superconductor from external magnetic field.

Substituting 1.10 and 1.14 into 1.9 gives the total electronic thermal conductivity;

$$k_{ele} = \frac{1}{3m}n_e\pi^2 K_B^2 T\tau - \frac{2}{3}\left(\frac{\pi^3\mu_0^2 k_B^2 T C\hbar^2 E_F^2\xi^2 H0\left\{1-(\frac{T}{T_c})^2\right\}J_z^2 exp\frac{2X}{\lambda_L}}{\emptyset_0 B e^7 B_y^2(0)}\right)\sum_J \frac{1+\exp(\frac{2\varepsilon_J}{k_B T})}{\sqrt{\Delta_{(0)}^2-\varepsilon_J^2}} \quad .... 1.15$$

Using Boltzmann's equation formalism in the relaxation-time approach, the thermal conductivity due to phonons heat carriers is given by (Hlubek, 2010);

$$k_{ph} = \frac{K_B}{2\pi^2 v}\left(\frac{K_B T}{\hbar}\right)^3\int_0^{\frac{\Theta_D}{T}}\tau(x)\frac{x^4\exp x}{(\exp x-1)^2}dx \quad ....1.16$$

Where, v is the phonon velocity, $\tau(x)$is phonon relaxation time, Θ_D is the Debye temperature and

$$x = \frac{\hbar\omega}{K_B T} \quad ....1.17$$

The total thermal conductivity in the superconducting medium is due to both electronic and phononic contributions, i.e,

$$k = k_{elec} + k_{ph} \quad ....1.18$$

Substituting equations 1.15 and 1.16 into 1.18 gives;

$$k=\frac{1}{3m}n_e\pi^2 K_B^2 T\tau - \frac{2}{3}\left(\frac{\pi^3\mu_0^2 k_B^2 T C\hbar^2 E_F^2\xi^2 H0\left\{1-(\frac{T}{T_c})^2\right\}J_z^2 exp\frac{2X}{\lambda_L}}{\emptyset_0 B e^7 B_y^2(0)}\right)\sum_J \frac{1+\exp(\frac{2\varepsilon_J}{k_B T})}{\sqrt{\Delta_{(0)}^2-\varepsilon_J^2}} + \frac{K_B}{2\pi^2 v}\left(\frac{K_B T}{\hbar}\right)^3\int_0^{\frac{\Theta_D}{T}}\tau(x)\frac{x^4\exp x}{(\exp x-1)^2}dx \quad ....1.19$$

2.2 Thermal diffusivity at the critical temperature of the superconductors.

Thermal diffusivity γ gives the rate at which heat is propagated through the superconducting medium during changes in temperature with respect to time as $\gamma = \frac{k}{\rho c}$

Substituting for k from equations 1.19 we get;

$$\gamma = \frac{\frac{1}{3m} n_e \pi^2 K_B^2 T\tau - \frac{2}{3}\left(\frac{\pi^3 \mu_0^2\, k_B^2 T C \hbar^2 E_F^2 \xi^2 \mathrm{H0}\left\{1-(\frac{T}{T_C})^2\right\} J_Z^2 exp\frac{2x}{\lambda_L}}{\emptyset_0 B e^7 B_y^2(0)}\right) \Sigma_J \frac{1+\exp\left(\frac{2\varepsilon_J}{k_B T}\right)}{\sqrt{\Delta_{(0)}^2 - \varepsilon_J^2}} + \frac{K_B}{2\pi^2 v}\left(\frac{K_B T}{\hbar}\right)^3 \int_0^{\frac{\Theta_D}{T}} \tau(x)\frac{x^4 e^x}{(e^x-1)^2}dx}{\rho c}$$

………………………. 1.20

The transition from the superconducting to normal state is a function of temperature and magnetic field. It is a reversible process that can be described by equilibrium thermodynamics. At H=H_C, the latent heat Q is absorbed which is exhibited as a result of the difference in internal energy of the normal and superconducting phases. This latent heat absorbed when superconductivity is destroyed by the application of magnetic field above the critical field is given by; (Kakani, 2017).

$$Q = -\frac{T}{4\pi} H(T)\frac{dH_{C(T)}}{dT} \text{……………1.21}$$

Where, H (T) is the applied magnetic field at the temperature T. The negative sign means that heat travels from a warmer region to a colder region.

To obtain the heat capacity C just before the transition from superconducting to normal state, the first derivative of equation 1.21 is obtained with respect to temperature T.

$$C = -\frac{1}{4\pi}\left\{TH(T)\frac{d^2H_C(T)}{dT^2} + T\frac{dH(T)}{dT}\frac{dH_C(T)}{dT} + H(T)\frac{dH_C(T)}{dT}\right\} \text{………………… 1.22}$$

C, is the amount of heat required to change the temperature of a given mass of a superconductor by 1K.

To obtain the amount of heat required to change a unit mass of the superconductor by 1K, c, is obtained from heat capacity C by equation 1.23;

$$c = \frac{C}{M} \text{ ………………………..4.23}$$

where, M is the mass of the superconducting material.

To obtain the specific heat capacity c, equation 1.23 is substituted into 1.22, to give;

$$c = -\frac{1}{4\pi M}\left\{TH(T)\frac{d^2H_C(T)}{dT^2} + T\frac{dH(T)}{dT}\frac{dH_C(T)}{dT} + H(T)\frac{dH_C(T)}{dT}\right\} \text{……1.24}$$

Substituting equation 1.24 into 1.20 gives thermal diffusivity **γ** at the transition point.

$$\gamma = \frac{M\left\{\frac{1}{3m} n_e \pi^2 K_B^2 T\tau - \frac{2}{3}\left(\frac{\pi^3 \mu_0^2\, k_B^2 T C \hbar^2 E_F^2 \xi^2 \mathrm{H0}\left\{1-(\frac{T}{T_C})^2\right\} J_Z^2 exp\frac{2x}{\lambda_L}}{\emptyset_0 B e^7 B_y^2(0)}\right) \Sigma_J \frac{1+\exp\left(\frac{2\varepsilon_J}{k_B T}\right)}{\sqrt{\Delta_{(0,O)}^2 - \varepsilon_J^2}} + \frac{K_B}{2\pi^2 v}\left(\frac{K_B T}{\hbar}\right)^3 \int_0^{\frac{\Theta_D}{T}} \tau(x)\frac{x^4 e^x}{(e^x-1)^2}dx\right\}}{-\frac{\rho}{4\pi}\left[TH(T)\frac{d^2H_C(T)}{dT^2} + T\frac{dH(T)}{dT}\frac{dH_C(T)}{dT} + H(T)\frac{dH_C(T)}{dT}\right]} \text{……………}$$

………1.25

At the transition point, T=T_C, and H= H_C =0, Applying this conditions to equation 1.25 and simplifying, gives;

$$\gamma = \frac{-\frac{4}{3}M\left(\frac{n_e \pi^3 K_B^2 T_C \tau}{m} + \frac{3K_B}{2\pi v}\left(\frac{K_B T_C}{\hbar}\right)^3 \int_0^{\frac{\Theta_D}{T_C}} \tau(x)\frac{x^4 \exp x}{(\exp x-1)^2}dx\right)}{\rho\, T_C\left[\frac{dH_C(T)}{dT}\right]^2} \text{………}$$

…………………..1.26

Substituting for H_C (T) from equation 1.5 into the denominator of 1.26 gives;

$$\gamma = \frac{-\frac{4}{3}M\left(\frac{n_e \pi^3 K_B^2 T_C \tau}{m} + \frac{3K_B}{2\pi v}\left(\frac{K_B T_C}{\hbar}\right)^3 \int_0^{\frac{\Theta_D}{T_C}} \tau(x)\frac{x^4 \exp x}{(\exp x-1)^2}dx\right)}{\rho\, T_C\left[\frac{d\left\{H_0\left[1-\left(\frac{T}{T_C}\right)^2\right]\right\}}{dT}\right]^2}$$

………………………. 1.27

Solving the expression at the denominator of equation 1.27 gives,

$$\rho\, T_C \left[\frac{d\left\{H_0\left[1-\left(\frac{T}{T_C}\right)^2\right]\right\}}{dT}\right]^2 =$$

$$\rho\, T_C \left[\frac{d\left\{H_0-H_O\frac{T^2}{T_C^2}\right\}}{dT}\right]^2 = \left(4H_0^2\rho\frac{1}{T_C}\right) \quad .1.28$$

Substituting equation 1.28 into the denominator of 1.27 gives,

$$\gamma = \frac{-\frac{4}{3}M\left(\frac{n_e\pi^3K_B^2T_C\tau}{m}+\frac{3K_B}{2\pi v}\left(\frac{K_BT_C}{\hbar}\right)^3\int_0^{\frac{\Theta_D}{T_C}}\tau(x)\frac{x^4\exp x}{(\exp x-1)^2}dx\right)}{4H_0^2\rho\frac{1}{T_C}}$$

……………………………………..1.29

The density ρ of a superconductor is its mass per unit volume;

$$\rho = \frac{M}{V} \quad \text{……………………………… 1.30}$$

Making V the subject of equation 1.30 and substituting in 1.29, then simplifying gives;

$$\gamma = -\frac{V}{3H_0^2}\left(\frac{n_e\pi^3K_B^2T_C^2\tau}{m} + \frac{3K_B^4}{2\pi v\hbar^3}T_C^4\int_0^{\frac{\Theta_D}{T_C}}\tau(x)\frac{x^4\exp x}{(\exp x-1)^2}dx\right)$$

…………………………..… 1.31

Equation 1.31 gives thermal diffusivity **γ** at the transition temperature T_C of the superconductor.

Considering the volume V of the superconductor to be, V= $1m^3$ and using the constants given in the table of constants and table 1.1, equation 1.31 is reduced to;

$$\gamma = -\left(\frac{0.36744T_C^2}{H_0^2} + \frac{2.073X10^{-7}T_C^4}{H_0^2}\int_0^{\frac{\Theta_D}{T_C}}\frac{x^4\exp x}{(\exp x-1)^2}dx\right) .1.32$$

Negative sign shows that heat diffuses from hotter area to colder area

3. RESULTS AND DISCUSSION

3.1 Essential parameters for mercury doped cuprate superconductors.

The table 1.1 shows the critical temperature, critical fields, Debye frequency and temperature of some mercury doped Cuprate superconductors that have been used in obtaining the results.

Cuprate formula	T_C (K)	Hc2 (T)	ω_D (Hz) X 10^{13}	Θ_D (K)
$HgBa_2CuO_4$	93	30.5	6.8	520
$HgBa_2CaCu_2O_8$	128	41.5	4.0	306
$HgBa_2Ca_2Cu_3O_{10}$	135	52.8	3.6	275

Table 1.1: The critical temperatures of some mercury doped Cuprate Superconductors, (Rapando,. *et al.*,2013), Grissonnanche,. *et al*., 2014)

3.2 Thermal diffusivity at various Critical temperatures of Superconductors.

From equation 1.32 and using table 1.1, we obtained variation of diffusivity with critical temperature as shown below;

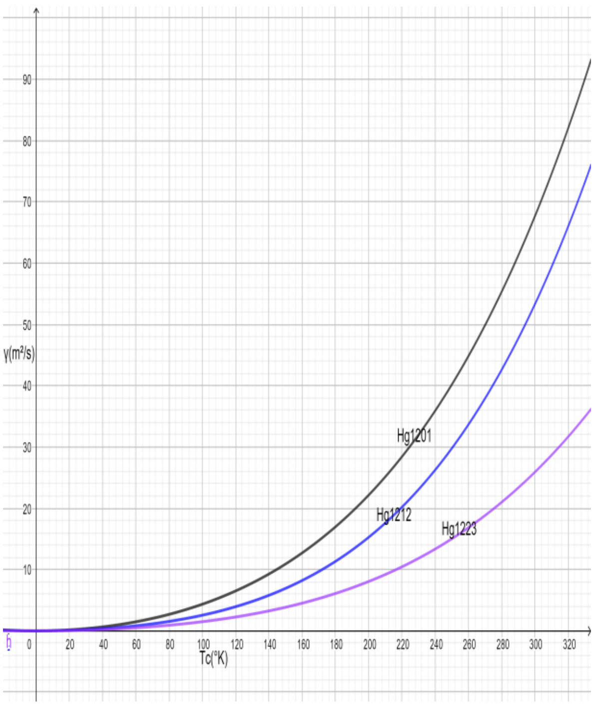

Figure 1.1: Variation of thermal diffusivity with critical temperatures of selected mercury doped Cuprate Superconductors.

The graphs shows exponential growth of thermal diffusivity with critical temperature of mercury-doped superconductors. The higher the diffusivity, the higher the critical temperature achievable. Critical temperatures approaching room (≈300K) are only possible if thermal diffusivity is highest. Hg1201 ($HgBa_2CuO_4$) is the best candidate to achieve this Tc since it shows the highest diffusivity in this region (68m^3/s) while Hg1223 give the lowest diffusivity of 26 m^3/s.

The inverse relation between diffusivity and the current experimental Tc for the three superconductors is a pointer to role played by doping in thermal diffusivity. Without undermining the importance of doping in enhancing superconductivity, our results show that high doping reduces diffusivity and consequently, the critical temperature. Though doping has raised the experimental Tc of Hg1223 to the highest of the three (135K), it has reduced its diffusivity thereby limiting its highest achievable Tc. Doping with oxygen atoms increases the Mott-insulation leading to localization of thermal charge carriers(electrons) hence reducing diffusivity. Low thermal diffusivity increases thermal energy accumulation which increases entropy and breaks Cooper pairs that enhance superconductivity. Our observation therefore suggests that an increase in doping level must be accompanied by addition of materials that enhance thermal diffusivity in order to achieve the highest Tc in any given superconductor. The values of diffusivity obtained in these Cuprates are lower than the thermal diffusivity of pure metals like diamond (1290 m^2/s) and most metals (23-116 m^2/s), but much higher than that of glass (0.56 m^2/s), ceramics (0.15 m^2/s) and various forms of plastics (0.44 m^2/s) at a temperature of about 20 ^{0}C, (Salazar, 2003).

4. CONCLUSION

We have shown that higher values of transition temperature for doped-mercury superconductors can be achieved if thermal diffusivity is enhanced in these materials. Oxygen doping level affects thermal diffusivity in such a way that high doping levels reduce thermal diffusivity and hence lowers the ability of the superconductor to a achieve the highest Tc. Room temperature superconductivity is possible in Hg1201 if the diffusivity is 68m^3/s and in Hg1223 if diffusivity is 26m^3/s.

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