A THEORETICAL ESTIMATION OF TEMPERATURE DEPENDENT RESISTIVITY OF ALKALI METAL DOPED FLUORIDE

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ABSTRACT

Using the theoretical formulism developed by Pintschovius[16], we have presented a method of evaluation of temperature dependent resistivity ρ_{e-ph} (electron-Phonon), ρ_{er} (Inter molecular Phonon), ρ_{ra} (Intra molecular Phonon), total resistivity $\rho_{(T)}$ and ρ_{diff} (Difference between theoretical-experimental) for K_3C_{60} fluoride. Our theoretical results are in good agreement with experimental data and also with other theoretical workers.

Key words: Normal state resistivity, Electron-phonon, Inter-molecular phonon, Intra-molecular phonon, Alkali metal doped fluoride, Electron doped cuprates, Dimensionally crossover.

INTRODUCTION

In this paper, we have presented the method of evaluation of temperature dependent resistivity due to electron-phonon interaction (ρ_{e-ph}), temperature variation of total resistivity $\rho_{(T)}$ and temperature variation of ρ_{diff} (measured ρ-calculated ρ) for K_3C_{60} fluoride. As we all know that electrical resistivity ρ can be caused by various scattering mechanism. An important mechanism is the electron-phonon interactions. In this mechanism electrons are scattered under the simultaneous excitations of phonons. The equally important mechanism is electron-electron interaction. The contribution of these two mechanisms[1,2] goes to zero as $T \rightarrow 0$.

In case of metal, electron-phonon scattering is the major source of temperature dependent resistivity. The other scattering mechanisms are electron impurities scattering due to defects, grain and disorder regions. Unfortunately, all these mechanisms give temperature independent contributions. For the evaluation of resistivity of alkali metal doped fluoride

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one uses zero temperature scattering rate related to upper critical magnetic field H_{c2} (0)[3], modified BCS theory and the use of Matsubara gap function[4], which uses to square well potential model. In these calculations the zero temperature resistivity is expressed as –

$$\rho(0) = 4\pi\tau^{*-1}\omega^{-2}_{p} \qquad\qquad \text{…(1)}$$

Here ω_p is the plasma frequency τ is the impurity scattering time. In this calculation, the zero temperature resistivity has been calculated by keeping the parameter[5]

$T_C = 22K$

$V_F = 1.9 \times 10^7$ cm/sec

$\omega_p = 1.2$ eV

H_{C2} (0) = 49 Tesla

$\tau = 1.23 \times 10^{-14}$ sec^{-1}

These all parameters are taken from the reference[6,7].

Our theoretical evaluated results of temperature variation resistivity $\rho_{e\text{-}eh}$ (due to electron-phonon), ρ_{er} (due to intermolecular phonon) and ρ_{ra} (due to intra molecular phonon), we have taken the intermolecular frequency $\omega_{er} = 9K$ and intramolecular frequency $\omega_{ra} = 1455K$. Our theoretical results show that ρ_{er} increases linearly with T and ρ_{ra} increases exponentially with T*. When these resistivities are combined together to calculated resultant resistivity $\rho_{e\text{-}eh}$ then it was found that $\rho_{e\text{-}eh}$ varies exponentially with low T and linearly with high T. Our other calculation ρ_{diff} shows that it has a power dependence of temperature as low T and it becomes almost saturated at high T.

Mathematical formula used in the evaluation

Now, one can estimate zero temperature limited resistivity with the help of zero temperature elastic scattering rate and plasma frequency. The zero temperature scattering rate is related through the upper critical magnetic field H_{C2} (0). Following the two square well analysis of Elishberg theory, Carbotte[8] suggested that the strong coupling correlations are important and a rescaling factor $(1 + \lambda)$ appears in the modified BCS results. The Mastubara gap function, which is related with upperand the factor critical magnetic field yields[9].

$$\left(\frac{1+\lambda}{\lambda-\mu^{*}}\right) = 2\pi\left(\frac{T}{T_c}\right)\sum_{m=0}^{N_c}\frac{1}{\chi_m^{-1}(\overline{\omega}_m)-(2\tau)^{-1}} \qquad\qquad \text{…(2)}$$

$\overline{\omega}_m$ Being the Mastubara frequency, within the standard two-square-well model is –

$$\overline{\omega}_m = \omega_m (1 + \lambda) + (2\tau)^{-1} (\text{sgn } \omega_m)$$

λ the electron-phonon coupling strength with cut off at N_C and the scattering time. In this approximation, N_C follows –

$$N_C = (^1/_2) [(^\omega/_{\pi T}) + 1] \qquad \qquad ...(3)$$

μ^* being the normalized Coulomb repulsive parameter and the factor χ_m appearing in (2) with,

$$\chi_m(\overline{\omega_m}) = \frac{2}{\sqrt{\xi}} \int_0^\infty \exp(-q^2) \tan^{-1}(\phi) dq$$

$$\phi = \frac{q\sqrt{\xi}*}{[(2m+1)\,\pi]\dfrac{T}{T_C} + \left[\dfrac{1}{2\tau*}\right]} \qquad \qquad ...(4)$$

The upper critical magnetic field is related through

$$\xi^* = \frac{1}{2} eH_{C2}^* v_F^{*2} \qquad \qquad ...(5)$$

The physical quantities appearing in (1) – (5) involve renormalized value as –

$$H_{C2}^* = \frac{H_{C2}}{(1+\lambda)\,T_C} \qquad \qquad ...(6)$$

$$v_F^* = \frac{v_F}{(1+\lambda)\,T_C} \qquad \qquad ...(7)$$

and impurity scattering time.

$$\tau^* = \frac{\tau}{(1+\lambda)\,T_C} \qquad \qquad ...(8)$$

The above derived equation differ from the BCS limit, as the renormalizations in ξ^*, v_F^*, H_{C2}^* and τ^* are introduced. These expressions are valid for any impurity concentration described in (1) - (5) by scattering time. In the present analysis, Pauli limit has been neglected as an approximation[9], due to relatively small value of $\dfrac{dH_{C2}}{dT\left[^1/_{[(1+\lambda)]}\right]}$ in alkali metal

intercalated fullerenes. In principle, the above approach describes quantitatively the renormalization of the physical properties due to electron-phonon interaction and is therefore reduced by $1+\lambda$.

The zero temperature-limited resistivity is expressed as –

$$\rho(0) = 4\pi\,\tau^{\bullet-1}\omega_p^{-2}$$

From the above, it is noticed that the determination of scattering rate essentially needs the Coulomb repulsive parameter, electron- phonon coupling strength, Fermi velocity, plasma frequency and upper critical magnetic field. This allows one to estimate the zero temperature-limited resistivity independently. One uses earlier deduced values[5] to estimate the zero temperature elastic scattering rate which is consistent as those derived from the superconducting fluctuation measurements[10]. It is attributed to the fact that the larger the electron mass, the smaller the plasma frequency and hence the zero temperature elastic scattering rate.

One has earlier estimated the zero temperature mean free path, ℓ about 3.4 nm which is highly sensitive for carrier scattering. One further finds that the product $K_F\ell$ (~ 17), seems to be much larger than unity indicates the metallic characteristics. It is worth to mention that the product, $\varepsilon F\,\tau \gg 1$, in the test material refers to the fact that the doped fluorides fall in the weak scattering limit. This is however, consistent with the s wave superconductors. With these parameters, one estimates zero temperature limited resistivity ($\rho_0 = 2.4$ mΩ cm) consistent with the single crystal result[10].

Normal state resistivity

To formulae a specific model, one starts with the general expression for the temperature dependent part of the resistivity[11]

$$\rho = \frac{3\pi}{\hbar e 2 v_F^2} \int_0^{2k_F} |v(q)|^2 \left\langle |S(q)|^2 \right\rangle \left(\frac{1}{2k_F}\right)^4 q^3 dq \qquad \dots(9)$$

V(q) is the Fourier transform of the potential associated with one lattice site and S(q) being the structure factor. Following the Debye model it takes the following form -

$$|S(q)|^2 = \frac{k_B T}{M v_S^2} f(x) \qquad \dots(10)$$

f(x) being the statistical factor and to -

$$f(x) = x[e^x - 1]^{-1} [1 - e^{-x}]^{-1} \qquad \ldots(11)$$

Thus the resistivity expression leads to

$$\rho \approx (\frac{3}{\hbar e^2 v^2}_F) \frac{K_\beta T}{Mv^2}_s \int_0^{2k_F} |v(q)|^2 [\frac{xq^3 dq}{(e^x - 1)(1 - e^{-x})}] \qquad \ldots(12)$$

v_s the sound velocity. Equation (12) in terms of intermolecular phonon contributation yields the Bloch Gruneisen function of temperature dependence resistivity *v*.

$$\rho_{er} = (T\theta_{er}) = 4A_{er}(^T/_{\theta_{er}})^4 \text{ x } T \int_0^{\theta_{er}/T} x^5 (e^x - 1)^{-1}(1 - ex)^{-1} \qquad \ldots(13)$$

Where x = $\hbar\omega/_{k_B}$ T.A_{er} being a constant of proportionality defined as -

$$A_{er} \cong (3\pi^2 e^2 kB)[K_F^2 v_F^2 L\hbar v_F^2 M]^{-1} \qquad \ldots(14)$$

In views of inelastic neutron scattering measurements, the phonon spectrum can be conveniently separated into two parts of phonon density of states[12,13]. It is natural to choose a model phonon spectrum consisting of two parts; an intermolecular phonon frequency, $\omega_{ra}(\theta_{er})$ and an intra molecular phonon frequency, $\omega_{ra}(\varphi_{ra})$. If the Matthiessen rule is obeyed, the resistivity may be represented as a sum $\rho(T) = \rho_0 + \rho_{e-ph}(T)$, where ρ_0 is the residual resistivity that does not depend on temperature. On the other hand, in case of the intra molecular phonon spectrum, $\rho_{ra}(T)$ may be described as follows

$$\rho_{ra} = (T, \theta_{ra}) = A_{ra} \theta_{ra}^2 T^{-1} [\exp(^{\theta_{ra}}/_T)^{-1}]^{-1} \times [1 - \exp(^{-\theta_{ra}}/_T)]^{-1} \qquad \ldots(15)$$

A_{ra} is defined analogously to (14). Finally the phonon resistivity reads -

$$\rho_{e-ph}(T) = \rho_{er}(T, \theta_{er}) + \rho_{ra}(T, \theta_{ra}) \qquad \ldots(16)$$

Henceforth, the total resistivity is now written as –

$$\rho(T, \theta_{er}, \theta_{ra}) = \rho_o + \rho_{er}(T, \theta_{er}) + \rho_{ra}(T, \theta_{ra})$$

$$= \rho_o + 4A_{er}(^T/_{\theta_{er}})^4 T \times \int_0^{\theta_{er}T} x^5 (e^x - 1)^{-1}(1 - e^{-x})^{-1} dx +$$

$$A_{ra}\theta_{ra}^2 T^{-1}[\exp(\theta_{ra}/T)^{-1}]^{-1}[1 - \exp(\theta_{ra}/T)^{-1} \qquad \ldots(17)$$

Though this is a purely phenomenological expression, it seems to provide a reasonable description of the available experimental data.

One also studied the temperature variation of different of resistivity.

$$\rho_{diff} = [\rho_{exp} - (\rho_o + \rho_{e\text{-}ph}\{\rho_{er} + \rho_{ra}\})] \qquad …(18)$$

where ρ_o – Is residual resistivity

$\rho_{e\text{-}ph}$ – Resistivity due to electron-phonon

ρ_{er} – Resistivity due to intermolecular phonon

ρ_{ra} – Resistivity due to intra molecular phonon

The resistivity has been studied theoretically by an approximate solution to the Boltzmann equation for the case of electron-phonon scattering mechanism[14]

$$\rho(T) = \frac{8\pi^2}{\omega_p^2 k_\beta T} \int_0^{\omega_{max}} d\omega \frac{\hbar\omega\alpha_{tr}^2 F(\omega)}{Cosh(\hbar\omega/k_\beta T) - 1} \qquad …(19)$$

where ω_p is the plasma frequency. In the above equation the transport coupling function can be replaced by the electron - phonon coupling for superconductivity[15]

$$\alpha^2 F(\omega(= \tfrac{1}{2}\sum_v \omega_v \lambda_v \delta(\omega - \omega_v) \qquad …(20)$$

Due to the factor in the denominator in equation (19) phonon with frequency much larger than T do not contribute. However, they give a linear contribution in T, if their energy is much smaller than k_β T.

RESULTS AND DISCUSSION

In this paper, using the theoretical formalism developed by Pintschovicus[16], we have presented the method of evaluation of temperature variation resistivity of alkali metal doped fluoride. We have evaluated temperature variation resistivity due to electron-phonon ($\rho_{e\text{-}ph}$), intermolecular phonon (ρ_{er}) and intra molecular phonon (ρ_{ra}), the results shown in table T_2. In this evaluation, we have used the value of intermolecular phonon ω_{re} = 9K and intra molecular phonon frequency ω_{ra} =1455K. Our theoretical result shows that ρ_{er} increasing

linearly with temperature and ρ_{ra} increasing exponentially with temperature. When both combined together then resultant resistivity ρ_{e-ph} varies exponentially at low temperature and linearly at high temperature. We have also calculated the total resistivity ρ (T) and compared our results with the experimental data. Our estimated values of ρ (T) are lower than the measured values. In this estimation, we have used the model parameter λ, μ^*, ν_F, ω_P, τ and ρ_0 which could be the reason of the lower valued of $\rho(T)$. We have also evaluated the temperature variation of ρ_{diff} for K_3C_{60} fluoride. From our evaluated results, it appears that ρ_{diff} has power temperature dependence at low T and almost saturated values at high T. The quadratic temperature dependence at low T is an indication of conventional electron-electron scattering. This is similar to electron doped cuprates[17]. The departure from T^2 dependence of ρ_{diff} is due to dimensionality cross over[18]. Thus in this paper, we conclude that for the estimation of temperature dependence resistivity in K_3C_{60}. The three scales of energy ω_{er}, ω_{ra} and ω_c (coulomb interaction) are of in same order and these are fully utilized in a model to estimate ρ which is sum of ρ_0, ρ_{e-ph} and ρ_{e-e}. Some recent[19-25] studies on fluorides also reveal similar type of behavior.

Table 1: Parameter used in the calculation

Tc = 22 K	ω_{er} = 9 K
V_F = 1.91 x 10^7 cm s^{-1}	ω_{re} = 1455 K
ω_p = 1.2 eV	ρ_o = 0.47 (mΩcm)
$HC_2(0)$ = 49 Tesla	

Table 2: Evaluated results of temperature variation of ρ_{e-ph}, ρ_{er} and ρ_{ra} for K_3C_{60} fluoride

T(K)	ρ_{e-ph} (mΩcm)	ρ_{er} (mΩcm)	ρ_{ra} (mΩcm)
0	0.0	0.0	0.0
20	0.02	0.02	0.0
40	0.14	0.15	0.0
50	0.16	0.17	0.0
100	0.22	0.25	0.0
200	0.78	0.50	0.22
300	2.5	0.70	1.52

Table 3: Evaluated results of temperature variation of total resistivity ρ(T) of K$_3$C$_{60}$

T(K)	ρ (T) (mΩcm)	
	Theory	**Expt.**
0	0.0	0.0
25	2.50	2.62
50	2.55	2.76
100	2.75	3.16
200	3.00	3.90
300	4.00	4.51

Table 4: Evaluated results of temperature variation of $\rho_{diff} = [\rho_{exp} - \rho_o + \rho_{e\text{-}ph} (= \rho_{er} + \rho_{ra})]$ for alkali metal doped fluoride K$_3$C$_{60}$

Temp. $T^2 (10^4 K^2)$	$\rho_{diff} = [\rho_{exp} - \rho_o + \rho_{e\text{-}ph} (= \rho_{er} + \rho_{ra})]$	
	Theoretical (mΩcm)	**Linear fit (mΩcm)**
0	0.125	0.132
1.0	0.110	0.156
2.0	0.268	0.295
3.0	0.455	0.462
4.0	0.622	0.656
5.0	0.668	0.575
6.0	0.585	0.853

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