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STUDY OF HIGH- TEMPERATURE SUPERCONDUCTORS AND THEORETICAL ESTIMATION OF ITS OPTICAL PARAMETERS

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Abstract: Frequency dependent scattering rate and effective mass of electron were evaluated for two high T_c-superconductors using extended Drude model at different temperatures. Our theoretically evaluated result for scattering rate is large and effective mass is small in comparison with experimental data for the given temperatures. However, the trend for both the scattering rate and effective mass are in agreement with the experimental data and also with other theoretical workers.

Keywords: Frequency dependent scattering rate, effective mass, High T_c- superconductor, optical parameters, Dirty limit , K-K relation.

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1. Introduction

The optical reflectivity measurement is a powerful probe for the study of the electronic structure of solids. It can provide much information on the conduction bands as well as valence bands of the crystals through inter band transition. It is a interesting problem for Bi-based cuprates. How the excitations within Bi_2-O2 layer affect those within Cu-O_2 layer and how the Optical transitions differ from those of Y-Ba-Cu-O and La-Sr-Cu-O. The optical reflectivity spectra of single crystal Bi- based cuprates $Bi_2Sr_2CaCu_2O_{8+x}$ and $Bi_2Sr_2CuO_{6+X}$ were measured [1] in a wide energy range from 0.5 to 40eV and analyzed through the Kramers-Kronig (KK) relation. The obtained spectra are different from other superconducting cuprates such as $(LaSr)_2CuO_4$ and YBa_2CuO_4 because of existence of characteristic BiO_2 layer. The optical excitation starts from 2eV or higher energy so it is unlikely that the electrons in the BiO_2 layer contribute to low energy excitations or dc conduction in this family of high –T_c superconductors.

Recently [2,3] there are two papers on the optical properties of high T_c superconductors $HgBa_2CuO_4$ (Hg-1201) (T_c=97K) and optimally doped $Bi_2Sr_2CaCu_2O_8$ (T_c=88K). In superconductor Hg-1201 in and out of plane optical spectra was presented. In plane normal incidence reflectivity measurement were performed on a Fourier transform spectrometer in the frequency range between 100-7000 cm^{-1} (12-870meV). Ellipsometric measurement were also made in the frequency range between 600 and 30,000 cm^{-1} (0.75 -3.72 eV). This measurement directly gives the real and imaginary parts of dielectric function $\varepsilon(\omega)$. Reflectivity was calculated from the pseudo dielectric function. In addition, the c-axis reflectivity $R_c(\omega)$ was measured on ac plane of different samples from 30 to 20,000cm^{-1}. The c-axis optical conductivity was obtained from Kramers- Kronig variational analysis [4].

In this paper, we report the evaluation of optical parameters namely the frequency dependent scattering rate $\frac{1}{\tau(\omega)}$ and effective mass $\frac{m^*(\omega)}{m_b}$ of Hg-1201 and Bi 2212. Using the extended Drude model [5] and taking the contribution from inter band transition in the infra red region $\varepsilon_{\infty,IR}$, we have evaluated the above optical parameters.

2. Materials and Methods

We have used extended Drude –Lorentz model [5] for the evaluation of frequency dependent optical parameters $\frac{1}{\tau(\omega)}$ and $\frac{m(\omega)}{m_b}$ .We have also used a term $\varepsilon_{\infty,IR}$ which is a contribution to the dielectric function in the infrared region arising from inter-band transitions. This term has not been taken into account earlier in the single component approach. Drude theory was the theory of non-interacting electrons which assumes a frequency independent scattering rate [$\frac{1}{\tau}$ =constant] is given by

$$\sigma(\omega) = \frac{1}{4\pi}\frac{\omega_p{}^2}{\frac{1}{\tau} - i\omega} \qquad (1)$$

ω_p is the bare plasma frequency of the free charge carriers. This assumption does not hold in the system where the charge carriers interact with bosonic spectrum or where strong correlations are important. In order to evaluate physical properties of high Tc superconductors Allen and Mikkelsen[5] extended the Drude model by including a frequency dependent scattering rate

$$\sigma(\omega,T) = \frac{1}{4\pi}\frac{\omega_p{}^2}{\frac{1}{\tau(\omega,T)} - i\omega\frac{m^*(\omega,T)}{m_b}} \qquad (2)$$

m^* is the effective mass and m_b is the band mass. $\frac{1}{\tau(\omega,T)} and \frac{m^*(\omega,T)}{m_b}$ obey Kramers –Kroing (KK) relations.[4] $\frac{1}{\tau(\omega,T)} and \frac{m^*(\omega,T)}{m_b}$ are simply related to the real and imaginary part of $\frac{1}{\sigma(\omega)}$.One can also express these terms in terms of dielectric function $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ where $\varepsilon_1(\omega) and \varepsilon_2(\omega)$ are the real and imaginary part of the dielectric function ,we have

$$\frac{1}{\tau(\omega)} = \frac{\omega_p{}^2}{\omega}\frac{\varepsilon_2(\omega)}{[\varepsilon_{\infty,IR} - \varepsilon_1(\omega)]^2 + \varepsilon_2{}^2(\omega)} \qquad (3)$$

$$\frac{m^*(\omega)}{m_b} = \frac{\omega_p{}^2}{\omega}\frac{[\varepsilon_{\infty,IR} - \varepsilon_1(\omega)]}{[\varepsilon_{\infty,IR} - \varepsilon_1(\omega)]^2 + \varepsilon_2{}^2(\omega)} \qquad (4)$$

where $\varepsilon_{\infty,IR}$ is the contribution to the dielectric function in the infrared region arising from inter-band transitions. The choice of $\varepsilon_{\infty,IR}$ is not so important at low energies where $|\varepsilon_1| \ll \varepsilon_{\infty,IR}$ but becomes important at high energies. One also writes

$$\varepsilon_{\infty,IR} = \varepsilon_\infty + \Sigma_j S_j \qquad (5a)$$

Where

$$S_j = \frac{\omega^2{}_{p,j}}{\omega^2{}_{0,j}} \qquad (5b)$$

These are the oscillator strength of the inter-band transition obtained from Drude Lorentz fit. The contribution to the dielectric function from the polarizability of oxygen is calculated using the Clausis-Mossotti relation[7,8]

$$\varepsilon_{\infty,IR} = 1 + \frac{4\pi N \frac{\alpha}{V}}{1 - \frac{4\pi}{3} N \frac{\alpha}{V}} = 1 + \frac{\alpha_0}{1 - \gamma\alpha_0} \qquad (6)$$

where N is the number of oxygen per unit cell. V is the unit volume and α is the polarizability of the oxygen atoms. $\alpha_0 = \frac{4\pi N\alpha}{V}$. For high T_c-superconductor $HgBa_2CuO_{4+\delta}$ (Tc =97K)putting α =3.88× 10^{-8} cm^3 and unit cell parameter for Hg -1201 of a×b×c =3.85×3.85×9.5Å and four oxygen atom per unit cell, we find $\varepsilon_{\infty,IR}$ =3.56 and for superconductor $Bi_2Sr_2CaCu_2O_8$ (Bi 2212, Tc =88K) $\varepsilon_{\infty,IR}$ =4.5.

The other important quantity is the in-plane reflectivity at low temperature. For frequency $\omega \prec 1/\tau$,one uses Hagen-Ruben approximation[9] to describe the reflectance

$$R(\omega) = 1 - 2\left(\frac{2\omega}{\pi\sigma_0}\right)^{1/2} \qquad (7)$$

where σ_0 is the dc conductivity. $\varepsilon_1(\omega) and \varepsilon_2(\omega)$ are calculated from K-K relation [10]

$$\varepsilon_1(\omega) - 1 = \frac{2}{\pi} P \int_0^\infty \left(\frac{x\varepsilon_2(\omega)}{x^2 - \omega^2}\right) dx \qquad (8a)$$

and

$$\varepsilon_2(\omega) = -\frac{2}{\pi} p \int_0^\infty \frac{\varepsilon_1(x)}{(x^2 - \omega^2)} dx + \frac{4\pi\sigma_0}{\omega} \qquad 8(b)$$

Equations 8(a) and 8(b) cannot be applied directly since both ε_1 and ε_2 depend on the unknown phase θ of the complex reflectivity

$$r = \frac{1 - \sqrt{\varepsilon}}{1 + \sqrt{\varepsilon}} = \sqrt{R} \exp(i\theta) \qquad 9(a)$$

R(ω) is the normal-incidence reflectivity

$$\ln r(\omega) = \ln\sqrt{R(\omega)} + i\theta(\omega) \qquad 9(b)$$

$$\theta(\omega) = -\frac{2\omega}{\pi} P \int_0^\infty \frac{\ln\sqrt{R(x)}}{(x^2 - \omega^2)} dx + \theta(0) \qquad 9(c)$$

These equations are used to compute $\theta(\omega)$ from $R(\omega)$. Now, one can restore dielectric function by inverting equation 9(a)

$$\varepsilon = \frac{(1 - r)^2}{(1 + r)^2} \qquad (10)$$

Now, one can also calculate the real part of the dielectric function in the superconducting state [11] by using the formulae

$$\varepsilon_1(\omega) = -\frac{\omega_{p_{1s}}{}^2}{\omega^2} \qquad (12)$$

Where $\omega_{p,s}$ is in-plane super fluid plasma frequency.[12] In case of superconductor

$HgBa_2CuO_{4+\delta}$ (T_c=97K). $\omega_{p,s}$ =9600 ± 400cm^{-1} (1.2 ± 0.05 eV). In case of superconductor $Bi_2Sr_2CaCu_2O_8$ (T_c=88K) $\omega_{p,s}$ =9500cm-^{1}.

3. Results and Discussions

We have evaluated frequency dependent scattering rate $\frac{1}{\tau(\omega)}$ using equation (3) at different temperature for two high T_c-superconductors $HgBa_2CuO_{4+\delta}$ (Tc=97K) and $Bi_2Sr_2CaCu_2O_8$ (T_c=88K). The results are shown in table T1 and T2 along with the experimental data [2,3,13]. Our theoretical results for $HgBa_2CuO_{4+\delta}$ indicate that the values of $\frac{1}{\tau(\omega)}$ is large in comparison to experimental data for all temperatures 250K, 200K, 100K and 50K between ω =100 to 4000cm^{-1} . On the other hand the values for $Bi_2Sr_2CaCu_2O_8$ is lower against the experimental data . In the experimental analysis of the $\frac{1}{\tau(\omega)}$ data [13], it was mentioned that scattering rate is strongly suppressed for temperatures below T_c which is indicative of the opening of the gap. ARPES [14] measurements on Hg -1201 show a maximum gap value, there is some uncertainty in this value because no quasi – particle peak is observed around the anti nodal direction [12]. From the optical measurements, it is difficult to extract the gap, s-wave BCS superconductor in the dirty limit show an onset in the absorption associated with the superconducting gap at 2Δ. It was observed that the onset seen in cuprates is shifted due to interaction of the electrons with the magnetic resonance [15]. Due to this, one feels that the evaluated results of $\frac{1}{\tau(\omega)}$ do not match with the magnitude of the experimental data. However the trend that $\frac{1}{\tau(\omega)}$ increases with ω for a given temperature has been noticed in our calculation for both superconductors Hg-1201 and Bi-2212. We have also evaluated frequency dependent effective mass $\frac{m^*(\omega)}{m_b}$ at different temperatures for both superconductors using equation (4). The results are shown in table T4 and T5. Our theoretically evaluated results show that up to ω = 600cm^{-1}, $\frac{m^*(\omega)}{m_b}$ increases with ω and after that it decreases with ω =4000 cm^{-1} . In case of superconductor Hg-1201 the magnitude of $\frac{m^*(\omega)}{m_b}$ is lower than the experimental data [2] and for superconductor Bi-2212 the evaluated results are larger with experimental data [13]. However the trend is in agreement with the experimental data [2,13]. The argument of this mismatch is the same as we have mentioned above. It has been pointed out that at onset of superconducting gap, K-K relations [4] gives maximum value $\frac{m^*(\omega)}{m_b}$. There is a quite uncertainty in the experimental data. In another work J. J. McGuire [16] studied the infra-red dissipation in the ab-plane scattering rate. They observed two separate effects. At high temperature there is a broad dispersion of scattering rate below $1000 cm^{-1}$ and at low temperature a sharp structure is seen which is associated with the scattering from a mode at $300 cm^{-1}$ in under doped high Tc- superconductor $Bi_2Sr_2CaCu_2O_8$ .. There are some calculations [17-31] which also reveals the same behavior. The various parameters used in the evaluation are shown in table T1.

CONCLUSION

In this paper we have estimated the optical parameters of high T_c superconductors. We have evaluated the optical effective mass and scattering rate of Hg-1201 and Bi-2212 superconductors. Our theoretical results are in satisfactory agreement with the experimental results although the magnitude does not match with the experimental data but the trend is the same.

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Table T1

$\varepsilon_\infty = 2.53$, $\varepsilon_{\infty,IR} = 3.56$ ($HgBa_2CuO_{4+\delta}$, Tc=97K)

$\varepsilon_{\infty,IR} = 4.5$ ($Bi_2Sr_2CaCu_2O_8$,Tc=88K)

$\omega_{p,s}$ (in plane super fluid plasma frequency) $=9600\pm400 cm^{-1}$ (1.2 ± 0.065 eV) $HgBa_2CuO_{4+\delta}$, Tc=97K) $\omega_{p,s} = 9500 cm^{-1}$ (Bi 2212)(Tc=88K)

Table T2

An evaluated result of frequency dependent scattering rate $[\tau(\omega)]^{-1}$ at different temperature for superconductor $HgBa_2CuO_{4+\delta}$

	$[\tau(\omega)]^{-1}$ x 10^3 cm^{-1}							
Wave number cm^{-1}	T=250K		200K		100K		50K	
	Theory	Expt	Theory	Expt	Theory	Expt	Theory	Expt
100	0.524	0.439	0.505	0.405	0.453	0.398	0.422	0.377
200	0.656	0.563	0.624	0.526	0.505	0.456	0.486	0.432
400	0.738	0.678	0.708	0.682	0.654	0.603	0.584	0.529
600	0.849	0.775	0.822	0.713	0.722	0.698	0.653	0.640
800	0.967	0.859	0.943	0.886	0.896	0.754	0.732	0.695
1000	1.128	1.098	1.106	0.986	0.954	0.863	0.853	0.782
1500	2.074	1.863	1.963	1.055	1.133	0.955	0.936	0.845
2000	2.365	2.059	2.124	1.354	1.586	1.124	1.139	0.957
3000	2.967	2.353	2.759	1.798	2.054	1.863	1.386	1.116
4000	3.547	2.958	3.128	2.154	2.846	2.058	1.754	1.458

Table T3

An evaluated result of frequency dependent scattering rate $[\tau(\omega)]^{-1}$ at different temperature for superconductor $Bi_2Sr_2CaCu_2O_8$ (2212) Tc=88K

	$[\tau(\omega)]^{-1}$ x 10^3 cm^{-1}							
Wave	T=300K		200K		150K		50K	
number cm^{-1}	Theory	Expt	Theory	Expt	Theory	Expt	Theory	Expt
100	0.183	0.204	0.154	0.162	0.098	0.107	0.055	0.067
200	0.196	0.223	0.167	0.174	0.115	0.112	0.074	0.088
400	0.206	0.236	0.188	0.193	0.128	0.137	0.083	0.097
500	0.217	0.247	0.195	0.205	0.139	0.144	0.094	0.105
600	0.222	0.255	0.204	0.214	0.146	0.152	0.106	0.112
800	0.238	0.263	0.215	0.222	0.155	0.167	0.118	0.126
1000	0.246	0.270	0.224	0.237	0.167	0.178	0.122	0.134
1500	0.287	0.292	0.249	0.256	0.199	0.207	0.144	0.155
1700	0.305	0.316	0.256	0.267	0.215	0.226	0.158	0.166
2000	0.346	0.352	0.264	0.277	0.224	0.237	0.167	0.174

Table T4

An evaluated result of frequency dependent effective mass $\frac{m^*(\omega)}{m_b}$ at different temperature for superconductor $HgBa_2CuO_{4+\delta}$ (Tc =97K)

	$\frac{m^*(\omega)}{m_b}$					
Wave	T=250K		200K		100K	
number cm^{-1}	Theory	Expt	Theory	Expt	Theory	Expt
100	3.20	3.52	2.53	2.66	2.46	2.54
200	3.86	3.97	2.95	3.03	2.58	2.68
400	4.52	4.72	3.84	3.64	2.67	2.77
600	5.50	5.80	4.50	4.72	2.86	2.94
800	4.30	4.54	4.28	4.34	2.48	2.53
1000	3.75	3.86	3.86	3.92	2.34	2.39
1500	3.22	3.57	3.67	3.84	2.21	2.26
2000	3.15	3.32	3.48	3.56	2.16	2.20
2500	2.86	2.97	3.22	3.37	2.10	2.15
3000	2.73	2.86	2.89	2.92	2.08	2.10
3500	2.67	2.74	2.75	2.84	2.05	2.09
4000	2.58	2.64	2.65	2.70	2.02	2.04

Table T5

An evaluated result of frequency dependent effective mass $\frac{m^*(\omega)}{m_b}$ at different temperature for superconductor $Bi_2Sr_2CaCu_2O_8$ (2212) Tc=88K

	$\frac{m^*(\omega)}{m_b}$					
Wave	T=300K		200K		150K	
number cm^{-1}	Theory	Expt	Theory	Expt	Theory	Expt
100	2.12	2.08	3.46	3.55	3.68	3.34
200	2.34	2.14	3.37	3.48	3.60	3.27
400	2.67	2.18	3.30	3.42	3.52	3.15
500	2.86	2.23	3.22	3.36	3.47	3.09
600	2.92	2.29	3.15	3.22	3.33	3.00
800	2.94	2.34	2.92	3.05	3.17	2.97
1000	2.99	2.38	2.75	2.95	3.09	2.84
1200	3.04	2.42	2.64	2.86	2.95	2.73
1500	3.07	2.56	2.53	2.74	2.87	2.65
1700	3.09	2.67	2.47	2.58	2.72	2.54
2000	3.12	2.75	2.38	2.49	2.63	2.44
3500	3.15	2.79	2.45	2.86	2.24	2.12
4000	3.23	2.98	2.54	2.36	2.44	2.29

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