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Multiband and mid-infrared optical conductivity in the normal state of $Mg(B_{1-x}C_x)_2$ superconductors

Namita Singh[1],
[1]Department of Physics, Ranchi College, Ranchi University, Ranchi - 834008, Jharkhand, India

R. Khenata[2]
[2]Département de Technologie, Université de Mascara, 29000 Mascara, Algeria.

Roopam Sharma[1,*],
[1]Department of Physics, Ranchi College, Ranchi University, Ranchi - 834008, Jharkhand, India

Dinesh Varshney[3, #]
[3]School of Physics, Vigyan Bhawan, Devi Ahilya University, Khandwa Road Campus, Indore-452001, India

Abstract**—** The frequency dependent optical conductivity σ (ω) of $Mg(B_{1-x}C_x)_2$, is discussed by considering spectral function for two-dimensional (2D) layered electron gas. Calculations of the σ(ω) have been made within the two component scheme: one is the coherent Drude carriers responsible for superconductivity and the other is incoherent motion of carriers from one site to other leads to a pairing between Drude carriers. The frequency dependent relaxation rates are expressed in terms of memory functions and the coherent Drude carriers from the effective interaction potential leads to a sharp peak at zero frequency and a long tail at higher frequencies, i.e. in the infrared region. Whereas the hopping of carriers from one site to other (incoherent motion of doped carriers) yields a peak value in the optical conductivity centred at mid infrared region. Both the Drude and hopping carriers in the lattice of $Mg(B_{1-x}C_x)_2$ will contribute to the optical process of conduction in B planes consistent with the results on optical conductivity in the mid infrared as well as infrared frequency regions as those revealed from experiments.

Keywords**—** ***Optical conductivity, layer interactions, Drude carriers, Hopping carriers, MgB*****$_2$**

I. INTRODUCTION

The announcement of superconductivity with a relatively high value transition temperature (T_c), multi-band nature and substantial electron-phonon interaction in MgB_2 showed a new impact in materials science and condensed matter theory [1]. Chemical substitution in MgB_2 is difficult and the successful cases such as substitution of Mg by Al and B with C have so far always suppressed T_c [2]. Examination of the multiple gap structures from tunneling spectroscopic and heat capacity measurements, suggests that it is the different parity of the σ and π bands that makes the interband impurity scattering to be negligible compared with intraband ones [3].

The grazing reflectivity spectra demonstrated a gradual increase at frequencies below 70 cm^{-1} with a maximum about 25-30 cm^{-1}, which might be considered as a sign of superconducting gap with a minimum value of about 3-4 meV [4]. Jung *et al.* showed far-infrared (IR) transmission optical spectrum on a *c*-axis oriented MgB_2 thin films and predicted the superconducting gap to be 700-1000 cm^{-1} and at 42 cm^{-1} (5.2 meV). The scattering rate from transmission spectra corresponding to low energy gap is about 700 - 1000 cm^{-1} [5]. The optical data on MgB_2 reveals that the real part of optical conductivity in low frequency regime exhibits (ω^{-1}) dependence rather than (ω^{-2}) dependence behaviour for photon energies larger than ($\omega \geq$ 5meV) consistent with the Fermi liquid approach [6]. Kakeshita *et al.* reported optical conductivity behaviour in spectral range 6 meV – 4.6 eV [7].

Electron-energy-loss-spectroscopy (EELS) has been used to probe the electronic structure of MgB_2 [8]. Zhukov *et al* [9] use random phase approximation (RPA) for the dielectric response as a function of momentum transfer and predict a very sharp plasmon (linear waves) mode (~ 3 eV) on the low energy side of momentum transfer. On the other hand, the reflectance of MgB_2 single crystal documents the *ab*-plane plasma edge with the plasma frequency of about 2 eV. A new step-like structure is observed in the polycrystalline sample from reflectance measurement at about 2.48- 2.73 eV [10].

The salient features of the optical conductivity from these experiments [4-10] are a narrow Drude peak with a small spectral weight, and a broad dome structure extending up to 1-1.5 eV. Another broad peak is centered at about 3.4 eV and at ~ 5.1 eV. The Lorentz components centered at about 3.4 eV and ~ 5 eV becomes narrower as temperature decreases [9]. The spectral weights of these anomalies become narrower as the temperature decreases and the origin of these deviations in the mid infrared region continues to hold interest on MgB_2.

The idea we have in our mind follows from the experimental suggestion that a mid-gap state is formed between the σ band and the π band with carrier doping and that this state entails a Fermi surface of the carriers responsible for the superconductivity. It is thus natural that the Drude component introduced above be identified with carriers in the mid-gap state. The evidence relating to participation of two species of carriers with different masses together with EELS and reflectance studies of MgB_2, have provided the motivation for present work. The first channel to the conductivity is the coherent Drude i. e., intraband component with temperature dependent damping. Second, the hopping of carriers from one band to another i.e., interband transitions.

II. THE MODEL

The diborides as MgB_2 $Mg(B_{0.95}C_{0.05})_2$ and $Mg(B_{0.9}C_{0.1})_2$ are known as a two-gap superconductor with several anomalous properties originating from the existence of two separates sheets of the Fermi surface, one quasi-2D (σ band) and second quasi-3D (π band). Two σ bands are formed by sp^2 hybrid orbitals stretched along boron-boron bonds and are two-dimensional with hole type carriers, while to that the two π bonds are formed by p_z orbitals of boron and are three-dimensional with electron as carriers in MgB_2. Furthermore, σ band holes are strongly coupled with optical E_{2g} phonon, while π band electrons are weakly coupled with phonons [11].

In view of the layered description of diborides, the effective dynamic interaction between the charge carriers is obtained in terms of the polarizability function $\Pi_j(q,\omega)$ for the carriers (σ and π band) in each boron layer

$$V_s(q,q_z;\omega) = 2\pi e^2 S(q,q_z)/[q\varepsilon(q,q_z;\omega)], \quad (1)$$

with $S(q, q_z)$ is the structure factor and response function in the notations of polarization function is [12]

$$\varepsilon(q,q_z;\omega) = \varepsilon_\infty + P(q,\omega)S(q,q_z) \quad (2)$$

with

$$P(q,\omega) = -2\pi e^2 \Pi(q,\omega)/q \ , \quad (3)$$

$\Pi(q,\omega)$ being polarizability function for two band of carriers. The charged quasi particles are being scattered by the optical phonons, the charge fluctuations as well impurities and posses a finite damping rate Σ. We can then calculate the optical conductivity as

$$\sigma(\omega) = \lim_{q\to 0}[\omega \operatorname{Im}\varepsilon(q,\omega)]/[4\pi] \quad (4)$$

The electronic polarizability within random phase approximation follows

$$P(q,\omega) = -2\pi e^2 Z^2 n_c q/[m^*_\mu \omega(\omega + i\Sigma(\omega)] \quad (5)$$

Ze being the sum of the ionic charge and the free electron charge, n_c is the 2D density and m_μ^* is the effective mass. The frequency dependent damping function or the inverse of relaxation time is denoted as Σ (ω).

The longitudinal dielectric response function for in-plane interactions is

$$\varepsilon(q,\omega) = \varepsilon_\infty - [2\pi Z^2 e^2 n_c q]/m^*_\mu \omega[\omega + i\,\Sigma(\omega)] \quad (6)$$

The frequency dependent damping function is

$$\Sigma_\mu(\omega) = \Sigma_\mu(0) + [\Sigma_\mu(\infty) - \Sigma_\mu(0)][-i\omega\Gamma_\mu(\omega)] \quad (7)$$

in terms of memory functions $\Gamma_\mu(\omega)$ and μ is either '0' or '1'. Furthermore, we denote $\Sigma_\mu(0) = \gamma_{\mu 0}$ and $\Sigma_\mu(\infty) = \gamma_{\mu\infty}$ as the low and high frequency limits of the damping function of the quasi particles, respectively [13]. In order to satisfy the requirements of causality, the memory functions are

$$\Gamma_\mu(\omega) = \int_0^\infty \Gamma'_\mu(t)e^{i\omega t}dt \quad (8)$$

where $\Gamma'_\mu(t = 0) = 1$ and $\Gamma'_\mu(t = \infty) = 0$. Using the Gaussian forms of Γ for memory function, namely by setting

$$\Gamma'_\mu(t) = \exp(-t^2/\gamma^2_{\mu c}) \quad (9)$$

$\gamma_{\mu c}$ being the characteristic relaxation rates. The notations $\gamma_{\mu 0}$ and $\gamma_{\mu\infty}$ are the inverse of life times of quasi particles, due to the scattering by external fields. While to that, $\gamma_{\mu c}$ associated with motion of scatterers. There are no constraints on ordering in magnitude among damping functions of quasi-particles.

III. RESULTS AND DISCUSSION

The effective mass of the carriers along the conducting boron plane is obtained from the electronic specific heat coefficient, γ, $m^{\sigma *} = 3\hbar^2\gamma d/\pi k_B^2$. While estimating the effective mass we consider the interplanar distance from the structural data, d = 3.525 (3.5164) Å and γ = 3.83 (2.8) mJ/mol/K^2 from the heat capacity measurement. The charge distribution in boron plane includes the ionic charge and the free electron charge, the ionic charge Ze being -2e. For the intralayer conduction i.e., Drude term we use $m^* = 3\, m_e$ for σ band and $m^* = m_e$ for π band carriers. We first deduce plasma frequency ω_p^σ (ω_p^π) and Fermi energy ε^π_F (ε^σ_F), respectively and is consistent with Band structure calculations [14] with average Fermi velocity as 8.2 × 10^7 cm sec^{-1} for π band carriers and 4.4 × 10^7 cm sec^{-1} for σ band carriers, respectively.

The optical conductivity sensitively depends on the values of relaxation rates. The quasi particle relaxation rates $\gamma_{\sigma 0}$, $\gamma_{\sigma\infty}$ ($\gamma_{\pi 0}$, $\gamma_{\pi\infty}$) for the Drude component dominates the low frequency behaviour of σ (ω) for σ (π) band. The relaxation rates are temperature dependent and for T = 300 K, we use $\gamma_{\sigma 0}$, $\gamma_{\sigma\infty}$ and $\gamma_{\sigma c}$ for σ band and $\gamma_{\pi 0}$, $\gamma_{\pi\infty}$ and $\gamma_{\pi c}$ for π band carriers. The results for the optical conductivity that corresponds to simple Drude model for σ and π band carriers are showed in Figure 1 (a, b and c) for pure and C doped MgB_2, $Mg(B_{0.95}C_{0.05})_2$ and $Mg(B_{0.9}C_{0.1})_2$. We find that a peak value of σ (ω) at zero frequency is observed which develops from the intralayer plasmon modes and a tail at higher frequencies. Both π and σ contributions are shown separately.

Turning to the second channel of conduction, i. e., the transfer of electrons from either B layer to Mg layer or vice versa through hopping. The relaxation rates γ_1 and $\gamma_{1\infty}$, for the hopping component dominating the mid infrared behaviour of the optical conductivity are roughly of the order of the intersite energies in the boron planes, their magnitude are thus estimated to be approximately 0.1–1.0 eV. The excitations may be substantiated by the phonon, or the hopping component. While to that the localised spin system or the lattice system are to be considered to interact with hopping component with characteristic rates γ_{1c}.

The magnitudes of these parameters lie in the range 0.01-0.5 eV. The relaxation rates at T = 300 K are chosen as $\gamma^h_{\sigma 0}$ $\gamma^h_{\sigma\infty}$ and $\gamma^h_{\sigma c}$ for σ band and $\gamma^h_{\pi 0}$, $\gamma^h_{\pi\infty}$ and $\gamma^h_{\pi c}$ for π band carriers, respectively. The relaxation times $1/\gamma^h_{\sigma 0}$ and $1/\gamma^h_{\sigma\infty}$ ($1/\gamma^h_{\pi 0}$ and $1/\gamma^h_{\pi\infty}$ for π band carriers) for σ band carriers, points to the process in which the carriers transfer from site to site through hopping.

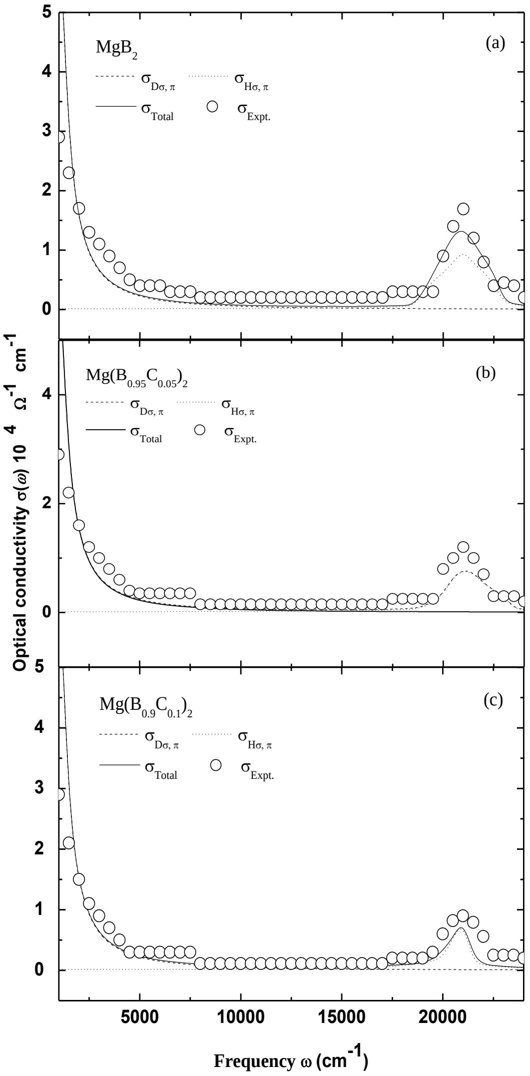

Fig.1.Variation of optical conductivity with frequency in MgB$_2$, Mg(B$_{0.95}$C$_{0.05}$)$_2$ and Mg(B$_{0.9}$C$_{0.1}$)$_2$. Experimental data is taken from [7] (Kakeshita *et al* 2006).

We plot the contribution of second channel for the optical conductivity in the Figure 1 (a, b and c) that corresponds to a non-Drude behaviour and a peak value at about 22000 cm^{-1} is obtained for MgB$_2$, Mg(B$_{0.95}$C$_{0.05}$)$_2$ and Mg(B$_{0.9}$C$_{0.1}$)$_2$. It may be pointed that the relaxation rates γ^h_0 and γ^h_∞ are involved in the hopping process and in MgB$_2$ superconductors, γ_{10} and $\gamma_{1\infty} \geq \varepsilon_F$, so the motion of electrons from one site to another site for interlayer transitions are no doubt hopping like. Both contributions are than clubbed and the resultant optical conductivity is plotted in Figure 1 (a, b and c) for pure and C doped MgB$_2$, Mg(B$_{0.95}$C$_{0.05}$)$_2$ and Mg(B$_{0.9}$C$_{0.1}$)$_2$ and is consistent with the data reported by Kakeshita *et al* on MgB$_2$ and C doped MgB$_2$ superconductors [7].

A representative value, $\gamma_{\sigma c}$ ($\gamma_{\pi c}$) = 400 (200) cm^{-1}, has thus been taken in the present study. Furthermore, the mean free path ℓ of the Drude carriers deduced from $\gamma_{\sigma 0}$ (1700 cm^{-1}) and the Fermi velocity ($v^{\sigma}_F \cong 2.7 \times 10^7$ cm sec^{-1}) for σ band and from $\gamma_{\pi 0}$ (1800 cm^{-1}) and the Fermi velocity ($v^{\pi}_F \cong 1.01 \times 10^8$ cm sec^{-1}) π band carriers yields a value of about 1.4 nm and 4.1 nm at T =300 K for σ and π band carriers, respectively.

We note that the relaxation rates γ^h_0 and γ^h_∞ satisfy a condition that $\gamma^h_{\sigma 0}$, $\gamma^h_{\sigma\infty}$ ($\gamma^h_{\pi 0}$, $\gamma^h_{\pi\infty}$) $\leq \varepsilon^{\sigma}_F$ (ε^{π}_F) reflects that the motion of the carriers is nodoubt hopping like. Furthermore, the mean free path L of the hopping carriers deduced from $\gamma^h_{\sigma 0}$ (1000 cm^{-1}) and the Fermi velocity ($v^{\sigma}_F \cong 2.7 \times 10^7$ cm sec^{-1}) for σ band and from $\gamma^h_{\pi 0}$ (1000 cm^{-1}) and the Fermi velocity ($v^{\pi}_F \cong 1.01 \times 10^8$ cm sec^{-1}) π band carriers yields a value of about 0.4 nm and 1.5 nm at T =300 K for σ and π band carriers, respectively. This may imply that the motion corresponds to the intersite hoping in the boron planes. It is thus anticipated that Fermi surface of the hopping component almost loses its sense.

IV. CONCLUSIONS

Precisely the two component model of conductivity, there are two channels of conductivity: the first is coherent Drude component with a temperature dependent damping function, and the second is the incoherent hopping component that is essentially temperature independent. The inclusion of the frequency dependent relaxation rates for the carriers is essential to account for the anomalous density fluctuations observed in the infrared region in the optical conductivity. We have quantitatively investigated the contributions to optical conductivity in the normal state following the RPA form of polarizability in the relaxation time approximation.

References

[1] J Nagamastu, N Nakagawa, T Muranaka, Y Zenitani and J Akimitsu *Nature* **410,** 63, (2001).

[2] M. Ortolani, D. Di Castro, P. Postorino, I. Pallecchi, M. Monni, M. Putti, and P. Dore *Phys. Rev. B* **71,** 172508, (2005).

[3] F. Bouquet, Y. Wang, I. Sheikin, T. Plackowski and A. Junod, *Phys. Rev. Lett.* **89,** 257001, (2002).

[4] B. Gorshunov, C. A. Kuntscher, P. Haas, M. Dressel, F. P. Mena, A. B. Kuzmenko, D. Marel, T. Muranaka and J. Akimitsu, *Eur. Phys. J.* B **21,** 159, (2001).

[5] J. H. Jung, K. W. Kim, H. J. Lee, M. W. Kim, T. W. Noh, W. N. Kang, H. J. Kim, E. M. Choi, C. U. Jung and S. I. Lee, *Phys. Rev.* B **65,** 052413, (2002).

[6] R. A. Kaindl, M. A. Carnahan, J. Orenstein, D. S. Chemla, H. M. Christen, H. Y. Zhai, M. Paranthaman and D. H. Lowndes, *Phys. Rev. Lett.* **88,** 027003, (2002).

[7] T. Kakeshita, S. Lee, and S. Tajima *Phys. Rev. Lett* 97, 37002, (2006).

[8] R. C. Yu, S. C. Li, Y. Q. Wang, X. Kong, J. L. Zhu, F. Y. Li, Z. X. Liu, X. F. Duan, Z. Zhang and C. Q. Jin, *Physica* C **363,** 184, (2001).

[9] V. P. Zhukov, V. M. Silkin, E. V. Chulkov and P. M. Echenique, *Phys. Rev.* B **64,** 180507(R), (2001).

[10] Y. Fudamoto and S. Lee, *Physical Rev.* B **68,** 184514, (2003).

[11] N. D. Markovskiy, J. A Munoz, M. S. Lucas, Chen W. Li, M. B. Stone, D. L. Abernathy and B. Fultz, *Physical Review B,* **83** 174301 (2011).

[12] D. Varshney, and R. K. Singh, *Phys. Rev. B.,* **52,** 7629, (1995).

[13] D. Varshney, G. S. Patel and R. K. Singh, *Supercond. Sci. Technol.,* **16,** 632, (2003).

[14] J. Kortus, I. I. Mazin, K. D. Bellashchenko, V. P. Antropov and L. L. Boyer *Phys. Rev. Lett.* **86,** 4656, (2001.