Interpretation of optical conductivity in normal state of Iron-Based Superconductors CeOFeAs

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Abstract. Quantitative analysis of the optical conductivity $\sigma(\omega)$ for the normal state of Iron-Based superconductors CeOFeAs have been made within the two-component scheme: one is the coherent Drude free carrier excitations and other is incoherent motion of carriers leading to a polaron formation, originated from inter and intra layer transitions of charge carriers. The model successfully accounts for the anomalies reported in the optical measurements for metallic state of the superconductors. 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 which is an indication of metallic conduction and a long tail at higher frequencies, i.e. in the infrared region. While to that the hopping of carriers from Fe to Fe in the FeAs layer and from FeAs layer to CeO layer (incoherent motion of carriers) yields two-peak value around 100 cm$^{-1}$ and 425 cm$^{-1}$ respectively in the optical conductivity centred at mid-infrared region. Both the Drude and hopping carriers contribute to the optical process of conduction in the iron-based superconductors and shows similar results on optical conductivity in the mid-infrared as well as infrared frequency regions as those revealed from experiments.

1. Introduction
The discovery of non-copper-based superconductors has attracted wide attention to elucidate the mechanism of superconductivity and to explore higher $T_c$ materials. It is believed that strong electron correlation and layered structures may play an important role. However, the $T_c$ of the non-copper-based superconductors is still lower than 40 K as predicted by BCS theory and experimental evidence. Recently, superconductivity in iron and nickel-based layered quaternary compounds has been reported: LaOFeP ($T_c = 4$ K) [1], LaONiP ($T_c = 3$ K) [2], Later on Kamihara et al. [3] found that by substituting P with As, and partially O with F in LaOFeP, the resultant material La(O$_{1-x}$F$_x$)FeAs ($x = 0.05-0.12$) became superconductive at 26K. The Fe$_2$As$_2$ layer, which is sandwiched between the La$_2$O$_2$ layers, serves as a carrier conduction path [1, 2] Thus, conduction carriers are two-dimensionally confined in the Fe$_2$As$_2$ layer, causing strong interactions among the electrons.

Chen et al. has presented the reflectance and conductivity spectra in a far-infrared region for CeOFeAs and LaOFeAs[4]. The reflectance below 400 cm$^{-1}$ is strongly suppressed at low frequency below the phase transition temperature, which is a strong indication for the formation of an energy gap. However, the low-frequency reflectance still increases fast towards unity at zero frequency, indicating a metallic behavior. Further more, the spin-density wave (SDW) partial gap is observed for
EuFeAs and LaOFeAs compounds [5]. The gap-like absorption peaks in the real part of conductivity for both the compounds scale with their respective $T_{SDW}$. The studies of reflectance and real part of optical conductivity of a single crystal of BaKFeAs [6] has shown that the absorption spectrum of this system consists of a noticeable Drude peak at low frequencies and a wide absorption band with maximum at 0.7 eV, which is attributed to carrier scattering by collective excitations with energies of the order of 25 meV and strongly temperature dependent coupling constant with carriers.

The aim of this paper is to explain theoretically some of the gross features observed in the experimental data on frequency dependent optical conductivity of iron-based superconductor, using a simple phenomenological model. The electronic dielectric function is evaluated following Random Phase approximation of polarizabilities. The first channel to the conductivity is the coherent Drude i.e., the intralayer component with temperature dependent damping. Secondly the hopping of carriers from one site to another (either Fe to Fe inter-layer hopping or from FeAs layer to CeO layer), small polaron as well as charge transfer.

2. The Model

The interaction potential in terms of dielectric function reads

$$V(q;\omega) = \frac{2\pi e^2}{q\varepsilon(q,\omega)}$$

(1)

$$\varepsilon(q,\omega) = \varepsilon_{\infty} + P(q,\omega).$$

(2)

The $\varepsilon(q,\omega)$ represents $\varepsilon_{ab}$ for interaction confined to $a$-$b$ plane. The charged quasi particles are being scattered by the optical phonons, the charge fluctuations as well impurities and possess a finite damping rate $\Sigma$. We can then calculate the optical conductivity as

$$\sigma(\omega) = \lim_{q\to0} \frac{\omega \text{Im}(\varepsilon(q,\omega))}{4\pi}$$

(3)

We shall now proceed to include polarizability of carriers in the long wavelength limit.

The electronic polarizability within random phase approximation for carriers follows

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

(4)

$Ze$ being the sum of the ionic charge and the free electron charge, $n_c$ is the 2D density and $m^*_\mu$ is the effective mass. The frequency dependent damping function is denoted as $\Sigma(\omega)$.

The model longitudinal dielectric response function for in-plane interactions as

$$\varepsilon(q,\omega) = \varepsilon_{\infty} - \frac{2\pi Z^2 e^2 n_c q}{m^*_\mu \delta(\omega + i\Sigma(\omega))},$$

(5)

The frequency dependent damping function of the quasi particles are expressed as

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

(6)

in terms of memory functions [7] $\Gamma_\mu(\omega)$ and $\mu$ is either ‘0’ or ‘1’. Furthermore, we denote $\Sigma_\mu(0) = \gamma_{\mu0}$ and $\Sigma_\mu(\infty) = \gamma_{\mu\infty}$ as the low and high frequency limits of the damping function of the quasi particles, respectively. In order to satisfy the requirements of causality, the memory functions are

$$\Gamma_\mu(\omega) = \int_0^\infty \Gamma_\mu(t)e^{i\omega t} dt,$$

(7)
where $\Gamma'_{\mu}(t = 0) = 1$ and $\Gamma'_{\mu}(t = \infty) = 0$. Using the Gaussian forms of $\Gamma$ for memory function,

$$\Gamma'_{\mu}(t) = \exp(-t^2 / \gamma^2_{\mu c}) \quad (8)$$

$\gamma_{\mu c}$ being the characteristic relaxation rates. Physically, $\gamma_{\mu 0}$ and $\gamma_{\mu c}$ are the inverse of life times of quasi particles, due to the scattering by external fields. While to that, $\gamma_{\mu c}$ are regarded as those associated with the motion of scatterers.

3. Results and Discussion

For the numerical calculation of the optical response of iron-based superconductors, we have used the realistic values of some physical parameters as follows: The effective mass of the electron along the conducting FeAs plane is $m^* = 17$ [8] which is consistent with the value deduced from electronic specific heat coefficient $\gamma = 11 \text{ mJ mol}^{-1} \text{K}^{-2}$. The behaviour of the multilayer systems critically depends on the electron density; we have used the charge carrier density $n_e = 1.7 \times 10^{21}$ electrons/cm$^3$ which is consistent with the Hall data [8]. The value of effective charge for conducting FeAs layer is used as $Ze = -2e$. The optical conductivity sensitively depends on the values of relaxation rates. The quasi particle relaxation rates $\gamma_{0c}, \gamma_{0x}$ for the Drude component dominates the low frequency behaviour of the optical conductivity. They represent the inverse of the lifetime of the carriers having a well-defined Fermi surface. The relaxation rates are temperature dependent and for $T = 170 \text{ K}$, we take $\gamma_{00} = 500 \text{ cm}^{-1}, \gamma_{0x} = 1000 \text{ cm}^{-1}$ and $\gamma_{0c} = 2200 \text{ cm}^{-1}$ for CeOFeAs superconductors, respectively.

Physically, the choice of the relaxation rates corresponds to the scattering process well described by phenomenological Drude model. However, the time $1/\gamma_{00}$ and $1/\gamma_{0c}$ for which the carriers can move freely without being scattered is much larger than the time $1/\gamma_{0c}$ in which the scatterers return to the initial state, the scatterers can respond to the motion of the carriers quickly enough. With these presumptions, we show in Figure 1, the results for the optical conductivity that corresponds to simple Drude model. We find from the present calculations that a peak value of $\sigma(\omega)$ at zero frequency is observed which develops from the free carrier plasmon modes and a tail at higher frequencies. The magnitude of the Drude peak is about 240 $\Omega^{-1}\text{cm}^{-1}$, which consistent with the experimental data [4] at $T = 170 \text{ K}$ in the CeOFeAs. Appearance of Drude peak at low frequency is an indication of metallic conduction in normal state of superconductor.

Switching to the second mode of conduction, i.e., the transfer of carriers (electrons) from site to site through hopping. We have considered first here the small polaron, originated from intra-layer transitions from Fe to Fe atom in FeAs layer which develops a peak value in optical conductivity at about 100 cm$^{-1}$. It is worth to comment that the effective mass $m^*$ for the hopping component is difficult to determine through the experiments due to shortness of the mean free path. The relaxation rates $\gamma_{10}$ and $\gamma_{1c}$ for the hopping component dominating the mid infrared behaviour of the optical conductivity. The characteristic rates $\gamma_{0c}$ are regarded as the motion of the excitations, which scatter the free carriers. The excitations may be substantiated by the phonon, the magnon or the hopping component. While to that the localised spin system or the lattice system are to be considered to interact with the hopping component with characteristic rates $\gamma_{1c}$. The relaxation rates at $T = 170 \text{ K}$ are chosen as $\gamma_{10} = 600 \text{ cm}^{-1}, \gamma_{1x} = 1000 \text{ cm}^{-1}$ and $\gamma_{1c} = 66000 \text{ cm}^{-1}$, respectively. Let us begin our discussion with the pronounced peak centered at 425 cm$^{-1}$ within the polaronic picture.

Another aspect of our analysis as shown in Figure 1 in the range from 300 cm$^{-1}$ to 500 cm$^{-1}$, the conductivity is dominated by the strong absorption at $\omega = 425 \text{ cm}^{-1}$. Incorporating an additional oscillator in the optical conductivity expression with $\gamma_{20} = 950 \text{ cm}^{-1}, \gamma_{2x} = 1000 \text{ cm}^{-1}$ and $\gamma_{2c} = 6200 \text{ cm}^{-1}$, respectively. The optical conductivity shows a prominent feature at about 425 cm$^{-1}$ and is associated with the interlayer charge-transfer transition from the CeO layer to FeAs layer. Both contributions are than clubbed and the resultant optical conductivity is plotted in Figure 2 along with the reported data on CeOFeAs superconductor [4] at $T = 170 \text{ K}$. We thus argued here that the low-frequency response should be coherent Drude peak and an incoherent mid-infrared absorption band, which takes account
Figure 1. Variation of optical conductivity with frequency in CeOFeAs.

of the two-component contributions, one is in between Fe-Fe and another feature is that the peak due to the CeO-FeAs charge-transfer excitations. We note that the relaxation rate $\gamma$ reflects that the motion of the carriers is hopping-like. It is thus anticipated that Fermi surface of the hopping component almost loses its sense.

4. Conclusion

The two-component model of optical conductivity presents two channels: the first is coherent Drude component with a temperature dependent damping function, leads to a sharp peak at zero frequency which is an indication of metallic conduction and the second is the incoherent hopping component. The hopping of carriers from Fe to Fe in the FeAs layer and from FeAs layer to CeO layer i.e. the incoherent motion of carriers yields two-peak value around 100 cm$^{-1}$ and 425 cm$^{-1}$ respectively in the optical conductivity centred at mid-infrared region.

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References
[1] Kamihara Y, Hiramatsu H, Hirano M, Kawamura R, Yanagi H, Kamiya T and Hosono H 2006 J. Am. Chem. Soc. 128 10012.
[2] Watanabe T, Yanagi H, Kamiya T, Kamihara Y, Hiramatsu H, Hirano M and Hosono H 2007 Inorg. Chem. 46 7719
[3] Kamihara Y, Watanabe T, Hirano M and Hosono H 2008 J. Am. Chem. Soc. 130 3296
[4] Chen G F, Li Z, Wu D, Li G, Hu W Z, Dong J, Zheng P, Luo J L and Wang N L 2008 Phys. Rev. Lett. 100 247002
[5] Wan-zheng HU, Dong J, Li G, Li Z, Zheng P, Chen G, Luo J, Wang N 2009 Front. Phys. China 4 459
[6] Yang J, Huusonen D, Nagel U, Room T, Ni N, Canfield P C, Bud’ko S L, Carbotte J P and Timusk T, arXiv: 0807.1040
[7] Varshney D, Patel G S, and Singh R K 2002 Supercond. Sci. Tech. 15 1617
[8] Sefat A S, McGuire M A, Sales B C, Jin R, Howe J Y and Mandrus D 2008 Phys. Rev. B 77 174503.