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Electron Behaviour of $(Nd_{0.33}Eu_{0.2}Gd_{0.47})Ba_2Cu_3O_y$ Studied by Infrared Measurements

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Optical properties of a $(Nd_{0.33}Eu_{0.2}Gd_{0.47})Ba_2Cu_3O_y$ single crystal are interpreted in terms of the extended Drude model.

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1. Introduction

We report here on the optical properties of a $(Nd_{0.33}Eu_{0.2}Gd_{0.47})Ba_2Cu_3O_y$ (NEG-123) single crystal interpreted in terms of the extended Drude model [1]. This work is an extension and continuation of our previous work [2].

The NEG-123 single crystal of approximately rectangular shape and $1.5 \times 2.0 \times 0.5$ mm^3 size was grown from melt in air and oxygenated at 683 K. Its reflectivity was measured from 50 to 8000 cm^{-1} in both the normal and superconducting states. The real parts of the dielectric function, ε_1, and the electrical conductivity, σ_1, were determined from the Kramers–Kronig (K–K) analysis of the reflectance data. The appropriate reflectance extrapolation in the low- and high-frequency range was done using $YBa_2Cu_3O_7$ (YBCO) data [3] from 8000 to 40000 cm^{-1}, $R \sim \omega^{-0.1}$ between 40000 and 10^6 cm^{-1} and $R \sim \omega^{-4}$ above 10^6 cm^{-1}[4]. The classical Drude–Lorentz model with constant parameters, describing free carriers, phonons and other spectral features, was used to fit the $\sigma_1(\omega)$ and $\varepsilon_1(\omega)$ functions resulting from K–K analysis, in both the normal and superconducting state [2]. Then, reflectivity was calculated from the functions and compared with the experimental data. This procedure was repeated until a self-consistent result was obtained.

We can subtract the contributions of phonons from $\sigma_1(\omega)$ and $\varepsilon_1(\omega)$ and the remaining part of dispersion describes the contribution of free carriers and middle infrared band. The phonons are modelled by a set of damped harmonic oscillators and no coupling between them and other excitations (e.g. electron–phonon) is assumed. The remaining part of conductivity, $\sigma_r = \sigma_{r1} + i\sigma_{r2}$, can be analyzed using an extended Drude (single-component) model, where the relation between the scattering rate $1/\tau(\omega)$, mass enhancement $m^*(\omega)/m$ [5] and conductivity is given

$$\frac{1}{\tau(\omega)} = \varepsilon_0\omega_p^2\left(\frac{\sigma_{r1}}{\sigma_{r1}^2+\sigma_{r2}^2}\right),$$

$$\frac{m^*(\omega)}{m} = \frac{\varepsilon_0\omega_p^2}{\omega}\left(\frac{\sigma_{r2}}{\sigma_{r1}^2+\sigma_{r2}^2}\right). \quad (1)$$

2. Results

Figure 1 shows the frequency dependence of $1/\tau(\omega)$ and $m^*(\omega)/m$ for four selected temperatures, calculated using Eq. (1). The $1/\tau(\omega)$ spectrum in Fig. 1a exhibits a significant peak in both the normal state and the superconducting state. The maximum of the peak in the normal state shifts with decreasing temperature from 298 cm^{-1} to 341 cm^{-1}. The height of the peak also increases on cooling from 1594 cm^{-1} to 2418 cm^{-1} and the peak sharpens with decreasing temperature. At 10 K, i.e. in the superconducting state, the peak position decreases to about 330 cm^{-1} and its height increases to about 2650 cm^{-1}. The peak further sharpens especially at its low-frequency side and $1/\tau(\omega)$ is practically zero below 200 cm^{-1}. For higher frequencies, above 900 cm^{-1}, the $1/\tau(\omega)$ spectrum exhibits a plateau, whose level increases from 350 to 530 cm^{-1} with decreasing temperature in the normal state and drops to 410 cm^{-1} in the superconducting state.

The mass enhancement, $m^*(\omega)/m$, in Fig. 1b exhibits a resonance-like frequency dependence and it becomes negative in a certain frequency range. The lower limit of this interval shifts with decreasing temperature from 290 to 380 cm^{-1} in the normal state and it drops to 350 cm^{-1} in the superconducting state, at $T = 10$ K. The upper limit of this region decreases on cooling from 930 to 810 cm^{-1} and it raises again slightly up to 830 cm^{-1} at $T = 10$ K.

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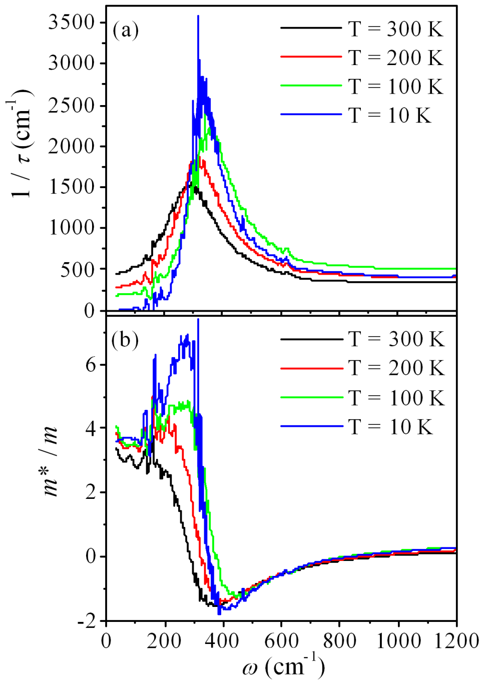

Fig. 1. Frequency dependence of relaxation time (a) and mass enhancement (b) of the crystal NEG-123.

The functions $1/\tau(\omega)$ and $m^*(\omega)/m$ substantially differ from those known from literature, where the data of more oxygenated YBCO crystals have been presented. The higher density of free carriers leads to a higher screening of spectral features like phonons and middle infrared absorption. In contrary, in our case the middle infrared absorption peak is strongly enhanced. It has character of a distinct resonance, which presses the function $m^*(\omega)/m$ downward, to negative values. All these features are consequence of the under-doped regime, where we expect the oxygen concentration, $y \approx 6.4$. This is also in agreement with the results of our previous work [2], where we reported a significant middle-infrared band in $R(\omega)$. We found that this band was composed of two highly damped Lorentz oscillators.

Similar effect like the negative $m^*(\omega)/m$ has been observed also in other materials. In heavy fermions ($UCu_{3.5}Pd_{1.5}$ [6] and $CeRu_4Sb_{12}$ [7]), the opening of hybridization gap due to mixing f-electrons and conducting carriers leads to a similar picture below a characteristic temperature.

Single-component model extended by the memory functions has been successfully used for YBCO [8, 9] with a high oxygen content. When the oxygen content decreases, the middle infrared absorption stands out from the Drude background and its resonance character prevails. As a consequence, $m^*(\omega)/m$ becomes negative and the single-component model has problems with describing this behaviour. The multi-component model could give more realistic picture, but it is not easy to separate contributions arising from free and bound carriers. On the other hand, the sharpening of the low-frequency side of the $1/\tau(\omega)$ peak illustrates opening of pseudogap on cooling.

3. Conclusions

In summary, we calculated the frequency dependences of scattering rate and mass enhancement in the crystal NEG-123 both in the normal and superconducting state. We found low contribution of free carriers and consequently enhanced role of mid-infrared band, which is not sufficiently screened out. On cooling the spectra of $\sigma_1(\omega)$ and $1/\tau(\omega)$ show a gap-like depression below 350 cm^{-1}, which is similar to opening of pseudogap.

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