Extra material for Localization by disorder in the infrared conductivity of $Y_{1-x}Pr_xBa_2Cu_3O_7$ films

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We present further quantitative analysis relating the optical conductivity in Pr substituted YBCO to its dc resistivity. We show that the charge density determined from the optical conductivity is in full agreement with the dc resisitivity if one considers localization of carriers and impurity scattering.

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We recently showed that the substitution of Y by Pr in $Y_{1-x}Pr_xBa_2Cu_3O_7$ leads to the localization of charge carriers on the *ab*-plane.[1] Upon doping, the Drude response in the optical conductivity of these materials gradually disappears to give origin to a peak centered around 300 cm^{-1} in the $x = 0.5$ sample. To describe the optical conductivity we developed a model based on localization by disorder introduced by the Pr atoms. This model is a shallow 2D potential with cylindrical symmetry having a radius of about the lattice parameter and a depth of about 1 eV. This potential leads to a weakly bound state of energy ε_0. The optical conductivity $\sigma_1(\omega)$ obtained from these states at $\omega \geq -\varepsilon_0/\hbar$ is given by

$$\sigma_L(\omega) = -A\varepsilon_0 \frac{\hbar\omega + \varepsilon_0}{(\hbar\omega)^3}, \qquad (1)$$

where A is a constant that depends on the concentration of bound states. The localized states give the dominant contribution to $\sigma_1(\omega \sim |\varepsilon_0|/\hbar)$ if $N_L > N_0 |\varepsilon_0| \tau/\hbar$ for $|\varepsilon_0|\tau/\hbar \ll 1$ or $N_L > N_0\hbar/|\varepsilon_0|\tau$ for $|\varepsilon_0|\tau/\hbar \gg 1$, where N_0 is the concentration of the mobile carriers participating in the Drude-like conductivity and $1/\tau$ is the scattering rate. The full conductivity of the system can then be described by three contributions to σ_1:

$$\sigma_1 = \sigma_L + \sigma_D + \sigma_{MIR}, \qquad (2)$$

σ_D being the Drude contribution and σ_{MIR} a phenomenological Lorentz oscillator that accounts for the incoherent conductivity. $\sigma_D + \sigma_{MIR}$ represents the Drude-like conductivity.

Figure 1 shows the fits obtained from this model to the $x = 0.4$ and $x = 0.5$ samples. In the latter the σ_D contribution is very small and has been neglected. The localization theory proposed also accounts for the very weak visibility of the localization peak in the $x = 0.4$ samples. The binding energy of the localized states is about 200 cm^{-1} in both samples. The low frequency scattering rate $(1/\tau)$ is 1000 cm^{-1} in the $x = 0.4$ sample and 2000 cm^{-1} in the $x = 0.5$ material. This gives us a localization peak visibility condition of $N_L/N_0 \gtrsim 0.1$. Using the values we get from the fits to N_L and N_0 we find a striking agreement between this condition and the optical conductivity.

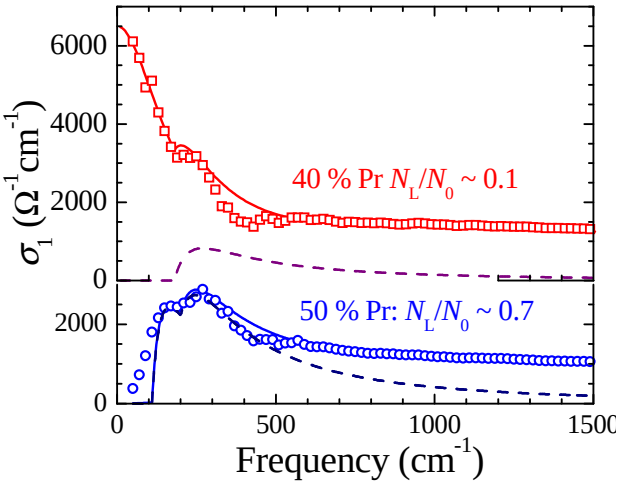

FIG. 1: Optical conductivity at 100 K for the $x = 0.4$ (top panel) and $x = 0.5$ (bottom panel) samples. The open symbols are the experimental data. The solid lines are fits using a Drude term for the free carriers, a mid-IR lorentian and the localization model described in this work. The dashed lines show the individual contribution of localized states to σ_1.

However we raised a question in our preceeding paper that was only answered qualitatively. The dc resitivity of the $x = 0.5$ sample is about 20 times higher than the one of YBCO. Knowing that $\sigma_0 = ne^2\tau/m$ (n is the charge density, e the electronic charge and m the electronic mass) and that τ does not vary more than a factor of two between the two samples, we would have expected that the decrease in σ_0 were represented by a decrease in n. As we described in our previous paper and as we show in Fig. 2 this is not the case. The evolution of the dc conductivity as a function of doping (triangles) is completely inconsistent with the evolution of the charge density obtained from the integral of the optical conductivity in both Pr substituted samples. This inconsistency can be overcome if we correct the dc values using Matthiessen's law

$$\frac{1}{\tau} = \frac{1}{\tau_0} + \frac{1}{\tau_1}. \qquad (3)$$

$1/\tau_0$ is the impurity scattering and is supposed to be temperature independent. In this case one should not

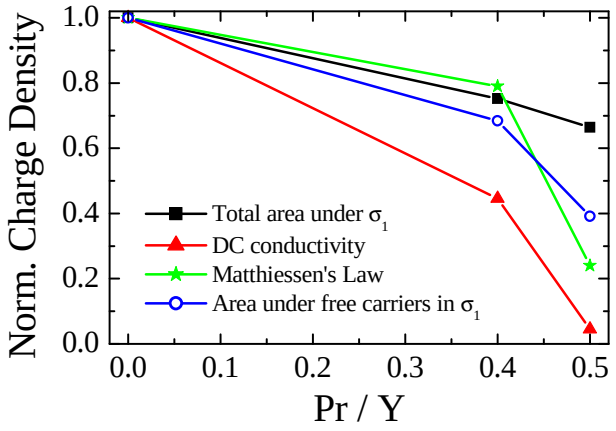

FIG. 2: Normalized charge density as a function of doping in Pr-YBCO. The values for $x \neq 0$ samples have been normalized by their corresponding quantities in pure YBCO.

compare the direct value of the dc conductivity with n but rather the slopes of the temperature dependent resistivities. By doing so we reconciled the values obtained from the optical conductivity to those from resisitivty in the $x = 0.4$ sample. This is shown by the stars in Fig. 2. However Matthiesen's law correction for the $x = 0.5$ material is far from being enough. This last issue is overcome if we consider that the localized states will not participate in the dc conductivity. When we calculate the charge density N_0 that do not include the localized carriers we obtain the curve described by the open circles. Comparing the open circles and the stars curves the agreement between the optical conductivity and the dc resistivity becomes clear.

In summary we show that a simple localization by disorder model can account for the optical conductivity of Pr substituted YBCO at any level of doping. The theoretical threshold for observation of the peak is compatible with the experimental data. The localization model quantitatively reconciles the high resistivity values measured in the $x = 0.5$ with the charge density obtained from the optical conductivity.

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