Optical properties and conductivity mechanism of $YBa_2CU_3O_{7-\delta}$ single crystals

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The reflection and absorption spectra of $YBa_2Cu_3O_{7-\delta}$ single crystals have been studied. A maximum has been observed at ~0.3 eV against the background Drude dependence of the optical-frequency conductivity $\sigma(\omega)$. The results are interpreted under the assumption that the light interacts with free and localized charge carriers.

Determining the particular features of the ensemble of charge carriers in the normal state is of interest for reaching an understanding of the nature of high-temperature superconductivity. Information of this sort can be extracted from the optical spectra in the region in which light interacts with charge carriers. With this goal in mind we have studied the reflection and absorption spectra of $YBa_2Cu_3O_{7-\delta}$ over the region 0.7–14 μm. The measurements were carried out at room temperature on a computer-controlled IKS-21 spectrometer.

The single crystals were grown by crystallization from a molten solution. They consisted of wafers with an area up to 4×4 mm^2 and a thickness of 20–200 μm. The samples quenched from 900 °C were of tetragonal symmetry with the lattice constants $a = 3.863$ Å and $c = 11.785$ Å. The symmetry of the single crystals quenched from temperatures below 800 °C was orthorhombic. The single crystals exhibiting the highest conductivity had the parameter values $c = 11.705$ Å, $a = 3.843$ Å and $b = 3.883$ Å. Polycrystalline samples with the same value of the lattice constant c have the values $a = 3.830$ Å and $b = 3.885$ Å, contain oxygen in an amount $\delta = 0.3$, and have[1] $T_c = 60$–70 K.

Using the $YBa_2Cu_3O_{7-\delta}$ single crystals, we measured the resistivity ρ. We calculated the anisotropy in ρ, and we calculated Hall effect. The resistance in the plane of the sample at room temperature was $\rho_{\|} = 10^{-3} - 10^{-1}$ $\Omega\cdot$cm. The anisotropy $\rho_{\|}/\rho_{\perp}$ was 20–30. The Hall mobility was $\mu \lesssim 0.1$ cm^2/(V·s). According to the experimental data on the resistance, the single crystals of tetragonal symmetry do not go into a superconducting state. Some of the single crystals of orthorhombic symmetry do undergo a superconducting transition, with $T_c = 60$–70 K. The resistivity of these samples decreases with decreasing temperature; near T_c there is a slight hump in $\rho(T)$.

A characteristic feature of the reflection spectra of all of the orthorhombic single crystals is a sharp increase in the reflection coefficient R with increasing wavelength of the incident light, starting at 0.9 μm (Fig. 1). This spectrum is similar to the reflection spectra of hot-pressed samples with various degrees of oxidation, for which an increase in R also begins at the same wavelength, regardless of the resistivity.[2] A similar dispersion of the reflection has been found[3] in the La-Sr-Cu-O superconducting system at

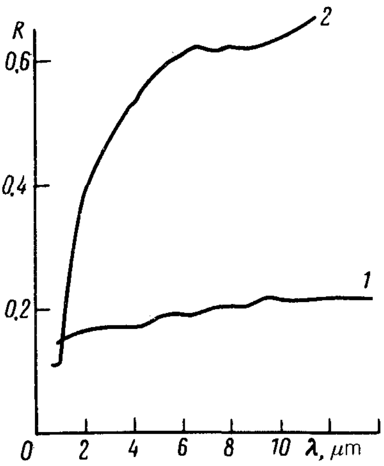

FIG. 1. Reflection spectra of $YBa_2Cu_3O_{7-\delta}$ single crystals of (1) tetragonal and (2) orthorhombic symmetry.

various Sr concentrations (at various values of the conductivity). It has been explained on the basis of a plasma edge of free charge carriers. In this case, however, the position of the reflection minimum should have depended strongly on the electrical conductivity of the sample. The structural feature observed in the dispersion of R for samples with various values of the electrical conductivity is characteristic of compounds with a low carrier mobility, e.g., $BaTiO_3$ (Ref. 4) and ferrite spinels.[5]

In the absorption spectra of the $YBa_2Cu_3O_{7-\delta}$ single crystals with a thickness of 20 μm, with various oxygen concentrations (Fig. 2), we see a maximum whose posi-

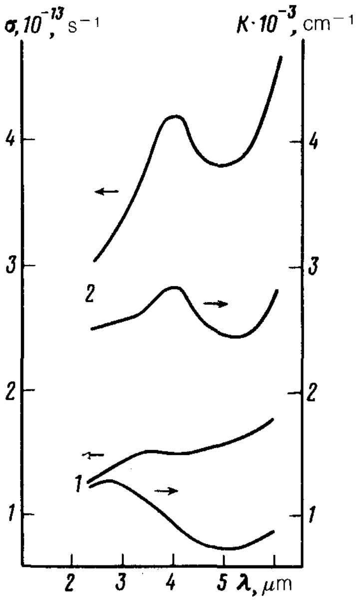

FIG. 2. Dispersion of the absorption coefficient (the reflection is taken into the account) and of the optical-frequency conductivity of $YBa_2Cu_3O_{7-\delta}$ single crystals with various oxygen concentrations. 1—$c = 11.750$ Å; 2—$c = 11.705$ Å.

tion depends on the oxygen concentration, which is characterized by the value of the lattice constant c. The shift of the absorption maximum and its intensification with increasing oxygen concentration, i.e., with decreasing number of defects, constitute evidence that this maximum is not an intracenter transition and is not associated with a defectiveness in terms of oxygen. It is apparently related to local excitations in the system of charge carriers. After a prolonged annealing in oxygen, the single crystals become opaque.

From the reflection and absorption spectra we calculated the optical constants: the absorption index k, the refractive index n, the real part (ε_1) and imaginary part (ε_2) of the dielectric constant, and the optical-frequency conductivity σ. The absorption and refractive indices increase with increasing wavelength; n varies from 4.5 to 8.0 over the interval from 2 to 6 μm. The real part of the dielectric constant, ε_1, increases from 20 to 60 under these conditions. The optical-frequency conductivity σ, shown in Fig. 2, is governed by at least two factors in the spectral range studied: The Drude contribution from free carriers and the absorption of light by localized carriers.

Several studies of the optical properties of the polycrystalline oxide superconductors $BaPb_xBi_{1-x}O_3$, $YBa_2Cu_3O_{7-\delta}$ (Ref. 6), $La_{2-x}Sr_xCuO_4$, and (rare-earth) $Ba_2Cu_3O_{7-\delta}$ (Ref. 7) have detected a maximum in the optical-frequency conductivity in the region 0.3–0.7 eV. This maximum is also noticeable in the $\sigma(\omega)$ spectra of a mosaic of $YBa_2Cu_3O_{7-\delta}$ single crystals.[8] Kamaras *et al.*[6] suggest that this maximum is due to electronic excitations which are responsible for the superconductivity in this compound. In our case, however, this maximum is also observed in nonsuperconducting samples. In the transmission spectra of oriented thin films with a high conductivity[9] (10^4 S/cm), this maximum is not observed. On the basis of that result, the authors assert that there are no excitations of any sort in the system of charge carriers in $YBa_2Cu_3O_{7-\delta}$. It is possible that the contribution of local excitations cannot be seen against the background of the strong Drude component in this case. The maximum in $\sigma(\omega)$ in the region of the interaction of the light with the charge carriers is therefore typical of oxide superconductors. It should be noted that a similar maximum in $\sigma(\omega)$ has been seen in other oxide compounds, not superconductors, with a low carrier mobility, e.g., in ferrites, where this maximum has been linked with an absorption by localized states of a polaron type.[5] In view of the general similarity of the optical spectra in the region in which the light interacts with the charge characters in $YBa_2Cu_3O_{7-\delta}$ and the $3d$ oxide compounds with a polaron conductivity, and also in view of the low carrier mobility in these compounds, one might suggest that polarons also exist in $YBa_2Cu_3O_{7-\delta}$. The position of the $\sigma(\omega)$ maximum and the magnitude of the limiting frequency of longitudinal optical vibrations, $\omega_0 = 600\ \text{cm}^{-1}$, lead to a value $\gamma = 2$ for the electron-phonon coupling parameter. The role played by polarons in mechanisms for high-temperature conductivity has been studied in several theoretical papers, e.g., Ref. 10.

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