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INTERBAND TRANSITIONS IN $\text{YBa}_2\text{Cu}_3\text{O}_7^*$

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PHYSICAL REVIEW

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Interband transitions in $\text{YBa}_2\text{Cu}_3\text{O}_7$

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Using Rotating Analyzer Ellipsometry we have measured all three components of the dielectric tensor of $\text{YBa}_2\text{Cu}_3\text{O}_7$ from the near-infrared to the vacuum-ultraviolet (0.7 – 24 eV). In the low energy region the spectra for $a - b$ polarization can be well modelled by a Drude free-carrier response with a frequency independent scattering rate. Below 10 eV we observe strongly anisotropic interband transitions involving the partially filled valence band and the conduction band. At higher energies the anisotropy becomes smaller. In that region we see two prominent double structures around 16 eV and 20 eV that we assign to transitions from lower lying bands with O s and Ba p character to states close to the Fermi level.

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I. INTRODUCTION

Ever since the discovery of high- T_c superconductors [1] optical experiments on these materials were stimulated by the hope to explain the pairing mechanism by the investigation of the normal state. Most work has been performed on the Y-Ba-cuprates, that do not only allow for a wide variety of atomic substitutions but also the modification of the crystal structure by including zero, one, or two Cu-O chains as structural units.

Due to their layered crystal structure almost all physical properties of these materials are strongly anisotropic. In addition to the strong $a - c$ anisotropy, the orthorhombic distortion of the materials containing chains introduces another $a - b$ anisotropy. Optical measurements of these materials are important for probing the combined density of states (and the corresponding matrix elements) as well as for the determination of transport properties or the existence of plasma edges. Unfortunately, the nature of the samples makes optical measurements of the anisotropic behavior of these materials difficult. They are usually grown as extremely thin platelets, leaving c -axis components of the optical properties experimentally inaccessible. Moreover, they often show heavy $a - b$ twinning (making measurements of the $a - b$ anisotropy impossible). Nevertheless work on the optical anisotropy of $\text{YBa}_2\text{Cu}_3\text{O}_7$, [2-5] can be found in the literature.

Most of the work on the optical $a - b$ anisotropy of $\text{YBa}_2\text{Cu}_3\text{O}_7$ [2-4] relates to the ir optical properties, either in connection with the detection of a superconducting

gap or with the low frequency transport properties.[2–4] In the vis-uv region, accurate measurements of the interband contribution to the reflectance are made difficult by stray light losses, and the $a - b$ anisotropy is obscured if the samples have been grown in Al_2O_3 crucibles and are therefore Al-contaminated (leading to a reduction of the orthorhombicity).

In this work we primarily focus on the a - b anisotropy of $\text{YBa}_2\text{Cu}_3\text{O}_7$. We present dielectric function data for $E \parallel a$ and $E \parallel b$ as obtained from ellipsometric measurements on untwinned $\text{YBa}_2\text{Cu}_3\text{O}_7$ single crystals. To gather information about free carriers, we extended the useful photon energy range of our ellipsometer down to 0.7 eV using a Ge-detector. This method should result in more accurate data in the plasmon-dominated region than the usual Drude fit to reflectance measurements, since two quantities (ϵ_1 and ϵ_2) are measured independently from each other.

Using synchrotron radiation we were able to get information about the interband transitions up to 24 eV. We also present data for the a - c anisotropy of $\text{YBa}_2\text{Cu}_3\text{O}_7$ that we obtained from ellipsometric measurements on a (110) oriented thin film. With the experimental data reported here we provide a complete dataset for comparison with calculations of the optical response of high T_c superconductors [6].

II. SAMPLE PREPARATION

A. Untwinned $\text{YBa}_2\text{Cu}_3\text{O}_7$ single crystals

The $\text{YBa}_2\text{Cu}_3\text{O}_7$ single crystal (2 mm $\times$ 3 mm in size) was grown in an Au-crucible employing a self-flux-method described elsewhere.[7] The crystal was then

mechanically detwinned by annealing it under uniaxial stress in flowing oxygen at around 450°C.[8] The success of this procedure was checked under a polarized light microscope. Recently, a group from John Hopkins University showed that gold might be incorporated into the crystal primarily on the chain Cu-sites.[9] Au-substitution should lead to an increase in T_c and possibly to increase disorder in the chains. However, resistivity measurements on similar crystals yielded resistivity anisotropies of $\frac{\rho_a}{\rho_b} \approx 1.5 \dots 1.8$ showing that chain fragments of sufficient length are still present.

The superconducting properties of our sample were checked with low field dc-magnetization measurements yielding a sharp transition at 91 K. Both [001] surfaces of the sample were polished to remove residues of flux as well as oxygen deficient material on the surface.

B. (110) oriented $\text{YBa}_2\text{Cu}_3\text{O}_7$ thin film

(110) oriented thin films of $\text{YBa}_2\text{Cu}_3\text{O}_7$ were grown on a (110) oriented SrTiO_3 substrate using the pulsed laser deposition technique [10]. The (110) orientation of the film with the $\text{YBa}_2\text{Cu}_3\text{O}_7$ c-axis aligned in the surface parallel to the [001] direction in the substrate surface was obtained by the combination of heteroepitaxial growth at low substrate temperatures ($\sim 600^\circ\text{C}$) and homoepitaxial growth at 720°C . X-ray diffraction measurements show the film to be (110) oriented with the volume fraction of the misoriented material being less than 1/1000. Raman measurements confirm this finding and allow to rule out the possibility of having obtained a (103) oriented sample (which grows under similar growth conditions and cannot be discriminated from

(110) by means of standard x-ray methods). The specimen shows the usual twinning. Resistivity measurements yield a sharp transition at 87 K. Details of the growth of the sample and its characterization can be found in Ref. [10]

III. EXPERIMENT

Rotating Analyzer Ellipsometry[11] was employed to measure the complex reflectance ratio

$$\rho = \frac{\rho_s}{\rho_p} \quad (1)$$

where ρ_p (ρ_s) is the complex reflectance for light polarized parallel (perpendicular) to the plane of incidence.

The standard energy range of our Rotating Analyzer Ellipsometer (1.66 – 5.66 eV) was extended into the near-ir down to 0.7 eV by using a liquid nitrogen cooled Ge detector (North-Coast EO817K) working in the energy range of approximately 0.7 – 2 eV, instead of the usual photomultiplier (PMT) with S-20 characteristics being optimized for the above mentioned energies (1.66 – 5.66 eV). Due to different time constants of the Ge detector and the S-20 PMT (the rather large time constant of the Ge detector causes a phase shift and a weakening of the AC part of the measured signal) the calibration parameters [12] need to be measured independently for both detectors. The measured spectra agree well in the overlap region of both detectors without any additional parameters used to match the spectra. Up to 5.66 eV the ellipsometric measurements were performed in air using these two detectors.

For the vacuum-uv region we made use of our newly developed synchrotron-UHV-ellipsometer [13] at the Seya-2m beamline at the BESSY electron storage ring in Berlin. Since the ellipsometric measurements in this apparatus require one order of magnitude more signal than in the ir-vis-uv setup, sample size and surface smoothness are crucial for the measurements in this energy regime.

Between 4 and 13 eV we believe that 2nd order light passing through the monochromator is intense enough to potentially contaminate the measurements. Below 9.5 eV, however, a MgF_2 Rochon prism is used as analyzer. Its optical absorption edge (~ 10 eV) serves as a filter for higher order radiation. Above that gap a triple-reflection gold polarizer has to be used transmitting first and second order alike. Beyond 26 eV the light intensity is decreased so drastically as compared to that observed at 13 eV that it can safely be neglected. Thus contamination of light above 13 eV by second order radiation should not be a major problem. Between 9.5 and 13 eV, however, we cannot rule out errors in the results due to the detection of second order light. For that reason no experimental data between 9.5 and 13 eV shall be displayed.

Ellipsometric measurements in the 1.66 – 5.66 eV region were performed before and after the in-vacuo measurements at the Synchrotron to check for changes in surface quality due to the exposure to vacuum. No sign for a change, in particular loss of oxygen (which would be detectable by the 4.1 eV peak [14]) could be noticed.

IV. EVALUATION OF THE EXPERIMENTAL DATA

For large dielectric function values and moderate anisotropies, the pseudodielectric function (i.e. the dielectric function calculated from the measured complex reflectance ratio assuming an isotropic, clean and homogeneous sample-ambient interface) is a good approximation for the dielectric tensor element along the line of intersection between plane of incidence and sample surface.[15] For the materials under consideration, this approximation needs to be improved by fitting the measured values to the ellipsometric equations for anisotropic samples.[16]

These considerations result in the following procedure: The complex reflectance of the (110)-oriented film is measured with the c -axis parallel and perpendicular to the plane of incidence. By fitting these experimental data to a uniaxial model (which is justified due to the presence of twinning) we obtain data for the dielectric tensor along c (ϵ^c) and perpendicular to c ($\epsilon^{\perp c}$).

The single crystal is also measured in two high-symmetry configurations, namely the a and b axes parallel to the plane of incidence. These two sets of data are fitted to a biaxial model together with ϵ^c as obtained from the film measurements as tabular (fixed) values. The ellipsometric measurements are, over the largest part of the spectral region, rather insensitive to the dielectric tensor component perpendicular to the sample surface (which can be seen by performing the fitting procedure for various data sets for ϵ^c). This fact makes a direct ellipsometric measurement of this quantity via variation of the angle of incidence not feasible but, on the other hand, justifies using c -axis data obtained from another sample. Above 10 eV, the pseudodielectric

function (as defined above) was assumed to be a sufficient approximation for the anisotropic behavior.

From the in-plane dielectric function $\epsilon^{a,b} = \epsilon_1^{a,b} + i\epsilon_2^{a,b}$ we calculate the effective number of electrons per unit cell, N_{eff}^i , by employing the sum rule

$$N_{eff}^{a,b}(\omega) = \frac{2mV_{cell} \cdot \epsilon_0}{\pi e^2} \int_0^\omega \epsilon_2^{a,b}(\omega') \cdot \omega' \cdot d\omega' \quad (2)$$

where e and m are the bare electronic charge and mass and V_{cell} is the volume of the unit cell. For the low-energy contribution to the integral in Eq. (2) we have used the Drude-Lorentz parametrized dielectric function

$$\epsilon(E) = \epsilon_\infty - \frac{E_p^2}{E(E + i\Gamma)} + \frac{F}{E_0^2 - E^2 - E_\gamma} \quad (3)$$

from recent infrared-ellipsometric measurements [17] with the parameters displayed in Table I.

V. RESULTS AND DISCUSSION

The dielectric tensor elements obtained in the above described fashion are presented in Figs. 1 – 5.

Let us first turn to the c -axis component of the dielectric function (in Figs. 3 and 6). At higher energies ($\hbar\omega > 6$ eV) the ϵ_2 spectrum, although still showing some structures, is remarkably flat and displays rather low absolute values. This becomes obvious when comparing the present c -axis data (obtained from the (110)-oriented film) with recently published [5] c -axis data taken on the side face on a layered ceramic sample (shown in Fig. 6): the two spectra have features at approximately the same

energies, but they are much weaker in Fig. 3. We think that this behavior is due to surface imperfections of the film sample, becoming only important in the vuv. Still, for the evaluation of ϵ^a and ϵ^b the dielectric function from Fig. 3 was used. Due to the low sensitivity of the in-plane measurements to the c -axis component, the error in the absolute values of $\epsilon_2^{a,b}$ should not be higher than 0.2.

The complex band structure of these materials and the resulting large number of critical points suggest that a peak in ϵ_2 does not correspond just to transitions around one single critical point. Thus fits of analytical lineshapes to the experimental data are only of limited physical value. In order to make the structure in the spectra more visible we have taken the derivative of the spectra with respect to the photon energy (shown in Figs. 7 – 9). The maxima of ϵ_2 are defined to represent “the peak position”. All observed peaks and their respective positions are listed in Table II. We have labeled the peaks $X_1, X_2, \dots, Y_1, Y_2, \dots, Z_1, \dots, Z_n$ where the capital letters designate the polarization and the subscript increases with energy. In order to be consistent with the nomenclature of a theoretical work on the following pages[6] some subscripts have been skipped.

The spectral range covered by the present work can be separated into 4 regimes:

(i) In the near-ir region the optical response is governed by transport properties and the free carrier contribution, although underlying interband transitions can be seen.

(ii) Above 1.3 eV the absorption due to the broadened plasma edge is sufficiently

small to clearly see interband transitions. Between 1.3 and 3 eV all the final states (apart from a possible hole pocket at the S -point) should be the three antibonding $pd\sigma$ -bands with $Cud-Op$ character that cross the Fermi energy.

(iii) For the next group of transitions between 3 and 10 eV the situation becomes more complicated, since transitions from the Fermi-level to higher lying bands are possible as well as transitions from the bottom of the valence band to states just above E_F .

(iv) Above 14 eV two new groups of transitions become possible, having the two well separated clusters of O 2s and Ba 5p bands as initial states.

The optical response (and its anisotropy) in the energy region below 3 eV (shown in an expanded plot in Fig. 10) has been discussed in some detail by Heyen et al. [18] in connection with resonant Raman experiments. These experiments however, were performed on *twinned* single crystals.

Within the spectral region under consideration (< 3 eV) the structure due to interband transitions are strongest for c -polarization of the incoming light. The strongest peak in ϵ_2^c is at 2.6 eV (Z_5) has additional structure on its low energy side which makes the peak rather asymmetric. Around 2.5 eV we observe peaks for the a - and b -polarizations (X_5 and Y_5), being somewhat larger for the latter case. The calculations in the work of Heyen et al. predict exactly this behavior and the authors assign Z_2 and Z_5 to a plane-to-chain transition, while X_5 and Y_5 are assigned to interband transitions within the CuO_2 planes. Other theoretical [19] and experimental [2] work

found in the literature is consistent with our data.

Above 3.5 eV, the observed structure gains complexity, since the Ba d and Y d (also Cu p) bands ≥ 3.5 eV above the Fermi-level become possible final state candidates. Clearly, detailed calculations are needed for the assignment of these features which shall be the goal of a separate publication on the following pages [6]. Let us, at this point, only focus on the experimental aspects of two of these peaks.

A feature at 4 eV in ϵ_2^a (X_6) and ϵ_2^b (Y_6) is very well suited to illustrate that the anisotropy of these materials may not always be safely neglected for ellipsometric measurements. These peaks are much more prominent in the initially obtained pseudodielectric function (as defined in Sec. IV) for the a or b axes in the plane of incidence. Part of the oscillator strength, however, stems from the step-like feature in ϵ_2^c (Z_6). After fitting the experimental data to the ellipsometric equations for an anisotropic material the peaks become weaker, in particular X_6 .

Another feature at 6 eV (X_8) shows a rather interesting behavior: it is present in ϵ_2^a only, thus possibly causing the different shape of the lower lying peaks X_7 and Y_7 . In a recent investigation of the optical response of (001) oriented $Y_{1-x}Pr_xBa_2Cu_3O_7$ films we have shown that the 6 eV feature vanishes when Y is replaced by Pr. Assuming that the most dramatic changes in band structure induced by this substitution occur close to ϵ_F we argue in [20] that either the initial or the final state for the corresponding transitions should be close to the Fermi level. This conclusion is in agreement with the assignment of a peak in EELS spectra at 5.6 eV [21] to a transition from the

Fermi level to Ba 5d states.

Full potential band structure calculations [22] provide some evidence for a band crossing ϵ_F at the S -point and having in part Ba p_x character, while another Ba p_y band is located just below ϵ_F . For a Ba d_{xy} final state an assignment of the X_8 peak to a Ba $5p \rightarrow$ Ba $5d$ at S could explain the observed anisotropy as the p_x state is not possible as initial state. Moreover, preliminary ellipsometric measurements on polycrystalline $\text{YBa}_2\text{Cu}_4\text{O}_8$ [23] show no peak at 6 eV. The most obvious difference between the published band structures of $\text{YBa}_2\text{Cu}_3\text{O}_7$ and $\text{YBa}_2\text{Cu}_4\text{O}_8$ [24,25] in the vicinity of the Fermi-level is the absence of the above mentioned hole pocket at the S point and it may be speculated whether this structure is linked to that detail of the electronic structure.

Let us now turn our attention to the optical response above 13.5 eV where it is only moderately anisotropic and, for this reason, only pseudodielectric functions are shown in Figs. 4 and 5. In this regime we observe, on a large background absorption, two complexes of peaks. A lower one, centered at 16 eV, appears as doublet in the b -direction (at 15.5 and 16.6 eV); only 16.6 eV structure can be seen in the ϵ_2^a spectrum. Around 19 eV we observe additional structure, at 18.5 eV in ϵ_2^a and at 19.5 eV in ϵ_2^b . The dielectric functions in this energy range are in qualitative agreement with optical conductivity data calculated from the electron energy loss-function measured on twinned $\text{YBa}_2\text{Cu}_3\text{O}_7$ samples [27]. The 16 eV doublet corresponds to the “I” peak in the results of Romberg et al., one of their spectra even displaying the doublet fine

structure. Their broad J -structure at 19 eV corresponds to a combination of our peaks at 18.5 and 19.5 eV. In this region we feel that both, the lower lying O 2s and Ba 5p bands become important. The O 2s levels are somewhat lower in energy than the Ba 5p states, yet the final O 2p states are at the Fermi-level as opposed to the empty Ba 5d bands that start some 3 eV above ϵ_F .

Due to the many possible critical points involving Ba bands the large background and the 19 eV peaks are likely to be Ba transitions, while the lower lying Y_{12} peak may be due to an O(4) 2s $\rightarrow$ O(4) 2p_y excitation at S (into the "hole pocket"). This assignment could explain why Y_{12} has no x polarized counterpart: The O(4) p_x-band is below ϵ_F . Recent band-structure calculations [28] strongly support this point.

Let us finally consider N_{eff} as defined in Eq. (2). To take into account the oscillator strength below 0.7 eV, we have made use of a parametrized dielectric function obtained from a Drude-Lorentz fit to our ellipsometric spectra in the energy range between 0.7 and 1.6 eV (see Tab. I). This model function was extrapolated to zero frequency and used in the far-ir region where no ellipsometric data are available.

More oscillator strength can be seen at lower energies along the b -direction than along a (not only due to the larger free carrier contribution along b); around 5 eV ϵ_2^a and ϵ_2^b intersect and thus the contribution to N_{eff}^a dominates above that energy. This behavior has been predicted by band structure calculations and shown to be an effect of the orthorhombic distortion. At 9.5 eV N_{eff} reaches the value of 8.6 (9.1) electrons/cell for a (b) polarization. Due to both, the inaccessible energy range in our

measurements (between 9.5 and 13.5 eV) as well as the reduced accuracy of our data above that gap, absolute numbers of N_{eff} are uncertain above 9.5 eV. Steps in N_{eff} , however may still be taken as an indicator for a new group of bands becoming important for electronic transitions. One such step is seen at ~ 14 eV indicating that above that energy the isolated lower lying bands with Ba 5*p* and O 2*s* character become possible initial states. Steps at lower energies are extremely weak, since the band width of the partially fitted Cu *d*- O *p* conduction band is large compared to the band gaps.

The total number of valence electrons in $\text{YBa}_2\text{Cu}_3\text{O}_7$ is 27 per unit cell, less than the maximum N_{eff} 's found in Fig. 11. Since the latter are still increasing beyond 20 eV, we conclude that some contribution of Ba 5*p* and O 2*s* semi-core electrons is required in order to explain the measured N_{eff} 's.

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FIGURES

FIG. 1. Real and imaginary part of the dielectric function as obtained from ellipsometric measurements on an untwinned $\text{YBa}_2\text{Cu}_3\text{O}_7$ single crystal for $E \parallel a$.

FIG. 2. Same as Fig. 1, but for $E \parallel b$.

FIG. 3. Real and imaginary part of the dielectric function for $E \parallel c$ as obtained from ellipsometric measurements on a (110) oriented thin film.

FIG. 4. High photon energy (≥ 12 eV) continuation of measurements of Fig. 1.

FIG. 5. High photon energy (≥ 12 eV) continuation of the measurements of Fig. 2.

FIG. 6. Same as Fig. 3, but obtained from the side face of a stack of single crystals.

FIG. 7. Derivative with respect to energy of the spectra shown in Fig. 1.

FIG. 8. Derivative with respect to energy of the spectra shown in Fig. 2.

FIG. 9. Derivative with respect to energy of the spectra shown in Fig. 3.

FIG. 10. Anisotropy of the imaginary part of the dielectric tensor in the region below 3.5 eV.

FIG. 11. Effective number of carriers N_{eff} vs. frequency calculated using the oscillator-strength sum-rule for ϵ_2^b (full line) ϵ_2^a (dashed line).

TABLES

TABLE I. Best-fit parameters of the Drude–Lorentz model of Eq. 3 for the dielectric function of $\text{YBa}_2\text{Cu}_3\text{O}_7$ along the a and b direction. The entries with no error margin were fixed in the fitting procedure.

	a	b
ϵ_∞	4.43 ± 0.15	5.32 ± 0.09
E_p (eV)	2.31 ± 0.07	3.47 ± 0.05
Γ (eV)	0.43 ± 0.02	0.27 ± 0.02
F (eV ²)	1.56 ± 0.15	2.40 ± 0.20
E_0 (eV)	1.4	1.4
γ (eV)	1.0	0.88 ± 0.10

TABLE II. Peaks (and their positions i.e. maxima) in the dielectric function as shown in Figs. 1 - 7.

<i>x</i> -polarization		<i>y</i> -polarization		<i>z</i> -polarization	
peak	position/eV	peak	position/eV	peak	position/eV
X_4	1.4	Y_4	1.4	Z_2	1.35
X_5	2.65	Y_5	2.6	Z_5	2.65
X_6	4.0	Y_6	4.05	Z_6	4.2
X_7	4.85	Y_7	4.55	Z_7	5.15
X_8	5.9				
X_{10}	7.65	Y_{11}	7.65		
X_{11}	8.2			Z_{11}	8.2

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