Specac

Application Note

How polarized radiation helps in studies of the properties of functional materials

Holographic Polarizers

INSIDE: Discover how polarized infrared light can probe anisotropy in conductive oxides.

Introduction

Transparent conductive oxides (TCO) represent a group of optically transparent and electrically conductive functional materials. Thin films of TCO are widely used in a number of electronic devices including touchscreens, liquid-crystal displays, OLEDs, and photovoltaics.

Zinc oxide (ZnO) is a typical TCO with a band gap of 3.43 eV, which enables its transparency in the IR spectral range. ZnO is characterized by the hexagonal wurtzite structure with a significant amount of anisotropy. ZnO belongs to materials with n-type conductivity.

The aim of this note is to demonstrate the possibilities of IR spectroscopy with polarized radiation in studying the vibrational and electrical transport properties of one of anisotropic TCO using the example of ZnO.

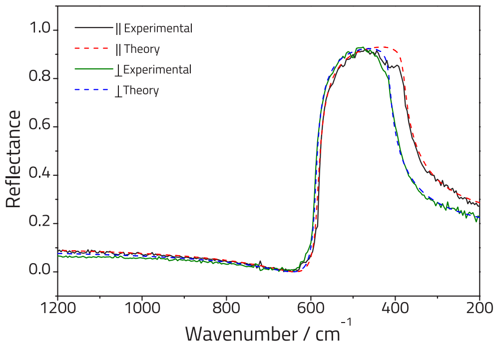

Figure 1: *Figure 1: Reflectance spectra of ZnO. $E_{||}C$: 1 – experimental, 2-theoretical; $E_{\perp}C$: 3 – experimental, 4- theoretical*

	Bonded electrons	Phonon mode			Free charge carriers	
	ε_∞	ν / cm^{-1}	γ / cm^{-1}	S	ν_p / cm^{-1}	γ_p / cm^{-1}
$E_{\|\|}C$	4.05	380	11.0	5.35	100	170
$E_{\perp}C$	3.62	414	9.8	3.6	90	150

Table 1: *Parameters of the model of the dielectric function for the ZnO sample*

Experimental

A ZnO single crystal in the form of a plate was used to obtain reflection spectra. The sample was oriented to the (100) crystallographic plane, so that the optical axis, C, was parallel to the sample's plane. Reflectance spectra were measured in the 200-1200 cm^{-1} (0.025-0.148 eV) range in an FTIR spectrometer. Since ZnO possesses an anisotropic crystal structure, a Specac KRS-5 holographic wire grid polarizer was used to obtain spectra for the parallel and perpendicular orientations of the electric field, E, with respect to the optical axis, C, of the ZnO crystal.

Results and Discussion

Reflectance spectra of the ZnO sample are shown in Figure 1. Both spectra have a similar shape, with broad lines between 300 and 600 cm^{-1} which are called Reststrahlen and appear due to lattice vibrations. In the range above 600 cm^{-1} reflectance is governed by the polarizability of bonded electrons. Free charge carriers are mainly responsible for the value of reflectance below 300 cm^{-1} and, therefore, this range is in our focus due to our interest in electrical transport properties of this material. It is noteworthy that the positions of the broad spectral lines, as well as values of reflectance in the frequency range below them, depend on the orientation of the sample. This qualitatively indicates the anisotropy of the vibrational and electrophysical properties of the studied TCO material.

A 2-parameter Drude model was fit to the experimentally obtained reflectance spectra. The model included one harmonic oscillator to describe phonon absorption, a constant to govern reflectance at high wavenumbers, and a contribution from free charge carriers. The values of these parameters are given in table 1, and the fit between the model and the spectra may be seen in figure 1.

These parameters quantitatively indicate anisotropy of vibrational properties, as well as pointing to the anisotropy in the electrical properties of the studied ZnO single crystal. Electrical properties, such as conductivity, concentration and mobility of free charge carriers can be calculated from the plasma frequency and damping (Fox 2006). To calculate these parameters, corresponding values of the effective electron mass have been taken from (Weiher 1966).

Electrical transport parameters which are displayed in the table 2 confirm the anisotropy of electrophysical properties of ZnO. The presence of free electrons in ZnO is explained by the presence of inter-site zinc atoms. This fact explains the correlation between the anisotropy of vibrational and electrophysical properties, which was revealed by using polarized radiation in our experiments.

Conclusion

Polarized FTIR reflectance spectroscopy provided a successful study of the electrical transport properties of ZnO, including conductivity, concentration of free charge carriers, and their mobility. The polarized radiation enabled us to study anisotropy in these properties of the ZnO sample. The method is shown to be quick, easy, and non-destructive.

References

Fox M (2006) Optical Properties of Solids. Oxford University Press

Weiher RL (1966) Optical Properties of Free Electrons in ZnO. Phys Rev 152:736–739 . doi: 10.1103/PhysRev.152.736

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