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Determination of anisotropic crystal optical properties using Mueller matrix spectroscopic ellipsometry

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Abstract

In this paper the Mueller matrix ellipsometry in the spectral range from 0.73 to 6.4 eV measured using dual rotating compensator ellipsometer RC2 (Woollam company) is applied to study anisotropic crystals. First we summarize the effects of optical anisotropy to Mueller matrix spectra. As an example of an uniaxial sample we have characterized a Rutile (TiO_2) tetragonal crystal. The optical axis of the sample is parallel to its surface. The sample is characterized at variable angle of incidence and variable azimuthal rotation angle. The Mueller matrix spectra are fitted to the model based on Kramers-Kronig consistent Basis spline and obtained optical functions are compared with tabulated data and ab-initio models based on first-principle calculated electronic structure.

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1. Introduction

Recent development in spectroscopic ellipsometry and ellipsometric instrumentation triggers wide applications of these techniques to characterize anisotropic nanostructures, periodic systems, and also crystals with reduced symmetry. Moreover, the Mueller matrix ellipsometry, i.e. measurement of all 15 reduced Mueller matrix elements, enables a complete characterization of reflection properties of the samples, including phenomena as mode conversion and depolarization [Garcia-Caurel (2013)]. The main task is usually to determine spectra of all components of the permittivity tensor from experimental data. The number of independent components depends on crystal symmetry. We summarize symmetries of the permittivity tensors for basic crystallographic groups and relate the permittivity tensor to observed Mueller matrices. The general method is applied to an uniaxial Rutile (TiO_2)

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crystal of tetragonal symmetry with the symmetry axis parallel to the plane of interface. The measured Mueller matrix spectra are fitted to a model consistent with Kramers-Kroning dispersion relations. Finaly, the obtained ordinary and extraordinary optical functions of Rutile are compared with the ab-initio calculations and peaks are related to the oxygen and titanum electrons.

2. Crystal symmetry and its optical properties

According to the Onsager relations, the permittivity tensor of a crystal should be symmetrical $\varepsilon_{ij} = \varepsilon_{ji}$, therefore in a general case of triclinic crystal symmetry, the material is described by 6 complex permittivity tensor components [Visnovsky (1986)]:

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{12} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{23} & \varepsilon_{13} & \varepsilon_{33} \end{pmatrix}. \quad (1)$$

For monoclinic crystals with c-axis paralell to the *z*-axis the permittivity tensor takes the form

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & 0 \\ \varepsilon_{12} & \varepsilon_{22} & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix} \quad (2)$$

and four independent components are necessary to describe the optical properties of absorbing crystals. We note that the real and imaginary parts of the tensors could be diagonalized by a rotation of the coordinate systems, however, the rotation is generally different for the real and imaginary parts of the tensors. The situation becomes more simple for orthorombic crystal symmetry for which we obtain diagonal form described by 3 independent permittivities components

$$\hat{\varepsilon} = \begin{pmatrix} \varepsilon_{11} & 0 & 0 \\ 0 & \varepsilon_{22} & 0 \\ 0 & 0 & \varepsilon_{33} \end{pmatrix}. \quad (3)$$

The tensor is diagonal if the symmetry axes of the orthorombic crystal are aligned with the coordinate system axes. In the case of uniaxial crystals, which includes tetragonal, trigonal and hexagonal symmetries, the form of the permittivity tensor (3) is simplified more by $\varepsilon_{11} = \varepsilon_{22.}$corresponding to the alignment of the symmmetry axis along the coordinate z-axis. The uniaxial medium is therefore described by two complex permittivities $\varepsilon_o = n_o^2 = \varepsilon_{11} = \varepsilon_{22}$and $\varepsilon_e = n_e^2 = \varepsilon_{33}$ denoted as the ordinary and extraordinary ones. Data presented in this paper deal with this kind of symmetry. The tensor (3) becomes even more simple for a cubic crystal, or isotropic medium, for which $\varepsilon_{11} = \varepsilon_{22} = \varepsilon_{33.}$
Permittivity tensor of generally oriented (rotated) medium can be obtained by trasnformation of the permittivity tensor by the formula $\varepsilon' = R^{-1}\varepsilon R$,where R is the rotation matrix. Therefore, for a general orientation of the uniaxial axis the off-diagonal components of the permittivity tensor are obtained. Reflection properties described by a Jones reflection matrix including reflection coefficients can be obtained using 4x4 matrix algebra [Yeh (1980), Visnovsky (1986)]. From the Jones reflection matrix one can calculate the Mueller matrix of the sample [Garcia-Caurel (2013), Postava (2002)].