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Temperature-dependent dispersion model of float zone crystalline silicon

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ABSTRACT

In this paper, we present the temperature dependent dispersion model of float zone crystalline silicon. The theoretical background for valence electronic excitations is introduced in the theoretical part of this paper. This model is based on application of sum rules and parametrization of transition strength functions corresponding to the individual elementary phonon and electronic excitations. The parameters of the model are determined by fitting ellipsometric and spectrophotometric experimental data in the spectral range from far infrared (70 cm^{-1}) to extreme ultraviolet (40 eV). The ellipsometric data were measured in the temperature range 5–700 K. The excitations of the valence electrons to the conduction band are divided into the indirect and direct electronic transitions. The indirect transitions are modeled by truncated Lorentzian terms, whereas the direct transitions are modeled using Gaussian broadened piecewise smooth functions representing 3D and 2D van Hove singularities modified by excitonic effects. Since the experimental data up to high energies (40 eV) are available, we are able to determine the value of the effective number of valence electrons. The Tauc–Lorentz dispersion model is used for modeling high energy electron excitations. Two slightly different values of the effective number of valence electrons are obtained for the Jellison–Modine (4.51) and Campi–Coriasso (4.37) parametrization. Our goal is to obtain the model of dielectric response of crystalline silicon which depends only on photon energy, temperature and small number of material parameters, *e.g.* the concentration of substituted carbon and interstitial oxygen. The model presented in this paper is accurate enough to replace tabulated values of c-Si optical constants used in the optical characterization of thin films diposited on silicon substrates. The spectral dependencies of the optical constants obtained in our work are compared to results obtained by other authors.

1. Introduction

Wafers of monocrystalline silicon (c-Si) are often used as a substrate for thin film growth in material science and microelectronics. The optical characterization of thin films is often performed in a wide temperature range from liquid helium temperature to high temperatures. In order to properly analyze the optical data of thin films, it is necessary to have a precise temperature-dependent optical constants of c-Si. Moreover, the optical constants of c-Si are dependent on dopants and impurities especially in the IR region [1–6]. The temperature dependence of the optical constants corresponding to various concentrations of dopants and impurities cannot be tabulated for practical purposes. It is necessary to point out that tabulation of the optical constants is impossible even when the wafers are taken from the same batch because the concentration of impurities and dopants varies along an ingot, *i.e.* for the individual wafers prepared from this ingot, but also in radial direction of this ingot. This means that individual pieces of silicon wafers will be slightly different.

During the last four years we have dealt with the problem of parametrization of the optical constants of c-Si [7,8]. At present we have a temperature dependent dispersion model expressing the dependence of dielectric response on the concentration of oxygen, carbon and phosphorus. This model is implemented in *newAD2* software [9].

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In this paper, we present an advanced temperature-dependent dispersion model of float zone (FZ) c-Si. Wafers of FZ c-Si represent the purest c-Si available on the market at reasonable prices. Note that, the presented dispersion model also depends on the density of substituted carbon atoms. This is important because carbon contaminant is present even in FZ c-Si, and its concentration can be different for each sample.

The model is developed on the basis of parametrizations of transition strength functions of individual elementary excitations normalized with respect to the sum-rule. The basic ideas were presented in our previous paper [10]. In that paper, only simple parametrizations describing individual elementary processes are discussed without details needed for construction of specific models. The current model is an improvement of the model of c-Si developed in [7] and [8].

In this paper, the theoretical background of the valence electron excitations will be presented in detail. The direct electronic transitions are modeled using Gaussian broadened piecewise smooth function representing 3D and 2D van Hove singularities (VHS) modified by many-body effects representing 3D Wannier and 2D Wannier (hyperbolic) excitons [11]. The indirect interband valence electron excitations are modeled using several truncated Lorentzian terms, the similar model was used for amorphous silicon [12,13]. Thermally induced free carrier contribution will be modeled by Drude-like term suggested in [10]. This contribution represents the indirect intraband transitions. The high energy electronic excitations will be modeled by two versions of Tauc–Lorentz model [14,15].

The theoretical background for phonon absorption will not be discussed in detail because it was already presented in our recent paper [8]. In that paper two-phonon absorption model suitable for describing absorption processes at the room temperature was presented. Above the room temperature the model anticipated lower absorption in the range 700–800 cm^{-1}. This discrepancy was explained by means of the absence of the higher order phonon absorption processes. This paper will show that the extension of the three-phonon absorption into this spectral range enables us to solve this problem.

The model will be applied to temperature-dependent ellipsometric data (5–700 K) combined with ellipsometric and spectrophotometric data obtained at the room temperature (300 K). It will be shown that the presented model describes experimental data very well, thus it is accurate enough for practical purposes.

2. Experiment

Dispersion parameters of the advanced dispersion model were determined by processing experimental data obtained on two samples. The sample #1 was a piece of double side polished FZ c-Si wafer. The sample #2 was cut from the same wafer as the sample #1, but the back side was covered by aluminum film. Both samples were cut along (100) plane from $5 \times 10^{13} cm^{-3}$ B-doped silicon with resistivity 80Ωcm. The thickness of the samples was 0.58 mm.

The instruments used for the experiment and the corresponding data sets are summarized in Table 1. It includes six table-top instruments covering the spectral range from the far IR to vacuum UV and the spectrophotometer at Elettra BEAR beamline [16,17] extending the spectral range of our measurements to the extreme UV.

The ellipsometric data measured at low temperatures were obtained with the help of a closed-cycle helium cryostat mounted on VASE and IR-VASE Woollam ellipsometers. The cryostat was equipped with an ultra-low vibration interface (ColdEdge Technologies) that allowed to decouple the mechanical vibrations from the Gifford-MacMahon refrigerator (Sumitomo Heavy Industries, Ltd.) from the optical experiment so that no impact from vibrations was noticed in the spectra. The cryostat used KBr windows for mid-infrared range or silica windows for higher frequencies and was working under 8×10^{-8} mbar and 3×10^{-8} mbar pressure, respectively, at 300 K. We have tested that under these conditions, there were no signatures of freezing of residual atmosphere on the sample. The high temperature IR ellipsometric data were measured using Instec heating cell (HC) with ZnSe windows under reduced pressure, whereas UV-VIS data were measured under vacuum with UVISEL2 VUV Horiba Jobin Yvon ellipsometer with heating stage. The spectrophotometric data were measured at the room temperature with Bruker Vertex 80v in vacuum, Perkin Elmer Lambda 1050 in air and Elettra BEAR beamline in the UHV condition.

Note that the ellipsometric quantities of sample #2 were also measured from the back side, *i.e.* from the side of aluminum film. The optical constants of alumina were determined from these measurements.

The ellipsometric quantities I_s, I_c and I_n used in this work correspond to the three independent elements of the normalized Mueller matrix M^0 of isotropic systems:

$$M^0 = \begin{pmatrix} 1 & -I_n & 0 & 0 \\ -I_n & 1 & 0 & 0 \\ 0 & 0 & I_c & I_s \\ 0 & 0 & -I_s & I_c \end{pmatrix}. \quad (1)$$

These three ellipsometric quantities are suitable for the description of depolarization effects, which must be taken into account, especially if the back side reflection is enhanced by the aluminum film. The degree of polarization P is related to these quantities as follows:

$$P = \sqrt{I_s^2 + I_c^2 + I_n^2}. \quad (2)$$

Note that without the reflection from the back side of the sample the ellipsometric data would not carry enough information about slight absorption occurring in the slab. The depolarization caused by the back side reflections is crucial for the determination of temperature dependencies of phonon absorption and temperature dependent indirect absorption edge in c-Si. The multiple back side reflection were calculated using Mueller matrix formalism. The fact that the beam is slightly shifted by each back side reflection and thus part of it falls outside of the aperture of the detector was also taken into account.

3. Data processing

All experimental data mentioned in Table 1 were fitted simultaneously in the *newAD2* software [9]. This software can fit together an arbitrary set of optical data using a single consistent model. All parameters of the model are fitted simultaneously and the weights of individual data sets are set such that the residual sum of squares is equally distributed between these data sets [19–21]. This equalization permits us to combine individual data sets with different spectral and angular densities from different spectral ranges obtained using different instruments exhibiting different systematic errors while keeping the sensitivity of the method to effects manifested in the individual data sets.

The influence of the native overlayer was taken into account as thin homogeneous film. The dielectric response of the overlayer was modeled by the universal dispersion model [21]. The thickness of the overlayer was determined separately for each measurement and each temperature. The dielectric function of the overlayer was assumed to be dependent on temperature, but it was assumed to be the same for different measurements. This is necessary because the native overlayer is an unstable system that depends on oxida-