Measurement of complex optical constants of a highly doped Si wafer using terahertz ellipsometry

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We propose and demonstrate a terahertz (THz) time-domain spectroscopy combined with ellipsometry. The complex optical constants of a Si wafer with low resistivity are deduced from the measurements of the wave forms of reflected s- and p-polarized THz pulses without reference measurement. The obtained dispersion of refractive index above ~0.2 THz shows good agreement with that predicted by the Drude theory. The complex optical constants deduced by the THz ellipsometry in the low-frequency region are strongly affected by the slight error of the ellipsometric angle originating mainly from the misalignment of the rotation angles of the polarizer and analyzer. © 2001 American Institute of Physics. [DOI: 10.1063/1.1427157]

Recently, many researchers have investigated the properties of materials in the THz region by using time-domain spectroscopy (TDS) systems equipped with femtosecond pulse lasers. However, since the usual TDS is carried out in the transmission configuration, the measurements on samples with low transmittance (<10−6), such as metals, highly doped semiconductors, and thick materials, are impossible. Therefore, reflection TDS has been reported by several groups. In order to obtain the complex reflectivity of the sample, the reflections from the sample and reference metal mirror should be measured. In the reflection TDS, it is difficult to measure the phase shift with sufficient accuracy due to the difficulty in placing the surfaces of the sample and reference mirror at the same position with sufficient precision (<1 μm). Even a slight error in the phase shift results in considerable error in determining the optical constants of the sample. To compensate for the misalignment of the relative position of the sample and reference mirror, adjustment of the relative position was done in the calculation of the optical constants to obtain the best fits to the Drude theory for doped silicon samples. Nashima, Takata, and Hangyo proposed an additional measurement by placing a plate with known refractive index in front of the sample to compensate for the misalignment.

On the other hand, reflection TDS without any reference measurement has been proposed by Li et al. The dielectric constants of films on the substrate have been deduced from the measurement of the incident angle dependence of the reflected THz wave form near the Brewster angle. However, in this TDS system, the alignment of each optical element and the sample is difficult, and the use of a large and expensive θ−2θ goniometer is needed. Dispersion of the complex reflection coefficient of an InSb sample has been measured without measuring the reflection from the reference mirror. In this case, the almost perfect sample reflection at high temperatures was used as a reference. Hence, no sample replacement is needed, however, the samples are restricted to narrow-gap semiconductors like InSb.

In this letter, we propose THz ellipsometry to measure the frequency dependence of the complex refractive index of samples without the reference measurement and without any assumptions. The effectiveness of this method is demonstrated by measuring the frequency dependence of the complex refractive index from 0.05 to 1.1 THz on a highly doped Si wafer.

The basic idea of THz ellipsometry is as follows. First, the wave forms of s- and p-polarized THz pulses reflected from the sample are measured at an incident angle. The measured wave forms are transformed to two complex spectra involving the amplitude and phase information by Fourier transformation. From these complex spectra, the frequency dependence of the ellipsometric angles is obtained. The frequency dependence of the complex refractive index is obtained from the ellipsometric angles by using the analysis of the conventional ellipsometry. Note the following facts regarding THz ellipsometry: (1) No assumptions on the characteristics of the sample are needed. (2) The frequency dependence of the complex optical constants of the sample is deduced from the measurement at an incident angle, that is, the measurement of the incident angle dependence is not needed. (3) In conventional spectroscopic ellipsometry, the intensity of the electromagnetic wave reflected from the sample is measured as a function of the rotation angle of the analyzer to obtain phase information. In THz ellipsometry, since the amplitude and phase of the THz pulse reflected from the sample are obtained at the same time, only two measurements of the s- and p-polarized THz pulses are needed. This is done by switching the rotation angle of the polarizer, that is, details of the rotation angle dependence are not needed.

Figure 1 shows a schematic diagram of the THz ellipsometry system we used. THz pulses were generated by a radiation antenna excited by a mode-locked Ti:sapphire laser with 80 fs time width pulses. The radiation antenna was a bow-tie-type photoconductive antenna with a 5 μm gap fabricated on a low-temperature-grown GaAs (LT-GaAs) thin film. The THz pulses generated by the radiation antenna were almost linearly polarized, and the radiation antenna was
oriented so that the amplitudes of s- and p-polarized THz pulses were equal. The s- or p-polarized THz pulse was extracted by a polarizer in front of the sample. The polarizer and analyzer placed in front of the detection antenna were wire grids of 10-μm-diam tungsten wires with a 25 μm spacing. The sample was mounted on a sample holder with an aperture diameter of 80 mm. The polarized THz pulses with an incident angle of 45° were reflected from the sample. The reflected THz pulses were focused on a detection antenna triggered by delayed laser pulses. The detection antenna was an incident angle of 45° were reflected from the sample. The aperture diameter of 80 mm. The polarized THz pulses with the normal reflection TDS measurement for the same sample were obtained by dividing the complex spectrum of the p-polarization by that of the s-polarization. Since there is no multiple reflection in the sample as mentioned above, the complex refractive index n−iκ is calculated by using equations for the bulk sample described by

\[ n^2 - k^2 = \sin^2 \theta_0 \left[ \frac{\tan^2 \theta_0 (\cos^2 2\varphi - \sin^2 2\varphi \sin^2 \Delta)}{(1 + \sin 2\varphi \cos \Delta)^2} \right], \tag{1} \]

\[ 2n\kappa = \sin^2 \theta_0 \frac{\tan^2 \theta_0 \sin 4\varphi \sin \Delta}{(1 + \sin 2\varphi \cos \Delta)^2}, \tag{2} \]

where θ₀ denotes the incident angle, and \( \tan \varphi = 1/\tan \Psi \).

The dots in Fig. 3 show the frequency dependence of the complex refractive index of the sample deduced from \( \tan \Psi(\omega) \) and \( \Delta(\omega) \) using Eqs. (1) and (2). In Fig. 3, the calculated values of the complex refractive index of the sample based on the Drude theory are also shown by solid and gray lines. In the calculation, we used the following parameters: electron effective mass \( m^* = 0.26m_0 \) (\( m_0 \) is the electron mass)\(^7\) and the dielectric constant of nondoped Si \( \epsilon_{\text{Si}} = 11.7 \),\(^8\) carrier density \( n = 4 \times 10^{16} \text{ cm}^{-3} \), and scattering rate \( 1/\tau = 1.59 \times 10^{-13} \text{ s}^{-1} \). The latter two were obtained by the normal reflection TDS measurement for the same sample used in this experiment.\(^4\) Above \( \sim 0.2 \text{ THz} \), n and κ obtained by the experiments gradually decrease with frequency, which are consistent with the values predicted by the Drude theory. Below \( \sim 0.2 \text{ THz} \), there exists a large discrepancy between the experimental and the calculated values.

The large discrepancy in the low-frequency region can be attributed to the fact that in determining the complex refractive index with large n and κ, the deduced values are affected strongly by the measurement error of \( \tan \Psi \). An equation for the electric field focused on the detection antenna is deduced by multiplying the Jones matrices of each optical element and the sample. Combining this equation with Eqs. (1) and (2), the complex refractive index is calculated for the case in which a small error is involved in the rotation angle of the analyzer. The polarization extinction ratio of the polarizer and analyzer is estimated to be less than \( 10^{-2} \) in the frequency region we investigated. We checked that the measurement error due to the polarization extinction ratio is smaller than that due to the error of the angular po-
sition of the polarizer, which is estimated to be within ±1°. Thus, in the following discussion, the effect of the polarization extinction ratio is neglected. Assuming that the error of the rotation angle of the polarizer $\delta \theta$ is 0.7°, the complex refractive index $n - i\kappa$ is calculated and is shown in Fig. 4. The value of $\delta \theta$ is determined so that the calculated values of $n$ and $\kappa$ well fit the experimental results. Note that the value of $\tan \Psi$ with $\delta \theta = 0.7^\circ$ has a uniform error of ~5% compared with the value with $\delta \theta = 0$ over the whole frequency range. In contrast, $\Delta$ is hardly affected by the value of $\delta \theta$. For comparison, the values of $n$ and $\kappa$ calculated from $\tan \Psi$ and $\Delta$ with and without the error ($\delta \theta = 0$) are shown in Fig. 4. As shown in Fig. 4, the frequency dependence of $n$ and $\kappa$ with $\delta \theta = 0.7^\circ$ shows large discrepancies with the value without the error in the low-frequency region.

For highly doped semiconductors, $n$ and $\kappa$ increase rapidly with decreasing the frequency. Therefore, in the low-frequency region, $\tan \Psi$ approaches 1 and the Brewster angle of the sample is increased. For the case in which $\tan \Psi$ approaches 1, a slight measurement error of $\tan \Psi$, mainly due to the misalignment of the rotation angle of the polarizer and analyzer, results in a large error and scattering of the complex refractive index. In order to improve the accuracy of the experimental data in the low-frequency region, it is necessary to measure at incident angles close to the Brewster angle of the sample and to reduce the misalignment of the rotation angle of the polarizer and analyzer.

In summary, we have applied ellipsometry to time-domain spectroscopy in the THz region. The complex optical constants of a Si wafer with low resistivity have been deduced. The obtained values show good agreement with the predictions of the Drude theory above ~0.2 THz. It is considered that the scattering of the experimental values below 0.2 THz originates from the fact that the slight error of $\tan \Psi$ becomes the large error of $n - i\kappa$ when $\tan \Psi$ approaches 1.

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