Characterization of the electrical properties and thickness of thin epitaxial semiconductor layers by THz reflection spectroscopy

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(Received 23 April 2001; accepted for publication 21 August 2001)

We have measured the dielectric properties and thickness of thin semiconductor epitaxy layers by the reflection of THz radiation from the surface of a two-layered semiconductor wafer. When reflecting from two interfaces the electromagnetic pulse has a destructive interference at a specific wavelength dependent on the thickness of the outer layer and its dielectric function. Near that frequency the reflection coefficient has a significant drop. By extending the incident pulse spectrum to include this interference frequency, a measurement of the thickness can be obtained together with a direct measurement of the carrier number density. By this technique epitaxy layers of thickness down to 15 μm are characterized.

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[DOI: 10.1063/1.1412574]

I. INTRODUCTION

It was recently demonstrated that properties of semiconductor crystals and other materials could be obtained by the analysis of THz reflection and transmission spectroscopy. The THz region of the electromagnetic spectrum proved to be very appropriate for the characterization of semiconductors since both the collision frequency and the plasma frequency, which are dependent on the carrier density in the relevant range of $10^{14} - 10^{20}$ cm$^{-3}$, are in the THz regime. There is a great interest in measuring properties of semiconductors with resistivities on the order of several $\Omega$ cm. The measurements clearly show that the dc resistivity calculated from the Drude theory and the reflection model (described below) is in agreement with measurements done by commercially available probes, even for epitaxy layers much thinner than the measuring wavelength. The thickness of the layers can be calculated accurately by using the strong dependence of the reflection coefficient on the frequency near the interference frequency that corresponds to the thickness and dielectric properties of the epitaxy layer. Reflection measurements are necessary when dealing with opaque samples. Furthermore, reflection measurements, as opposed to transmission, are advantageous when analyzed in the time domain.

II. THEORETICAL MODEL

Our calculations were based on a generalization of the Fresnel equations for the reflection of electromagnetic waves. The reflection from a three-layer system (layers denoted as 1, 2 and 3, 1 being the medium where the pulse propagates to and from the sample) can be written as

$$R_{123} = \frac{R_{12} + R_{23}e^{2i\beta_2}}{1 + R_{12}R_{23}e^{2i\beta_2}},$$

where $R_{jk}$ is the frequency dependent reflection coefficient of the $j-k$ surface, and $\beta_2 = (2\pi/\lambda_0)n_2h_2 \cos \theta_2$ is the phase accumulated from one trip across the middle layer (2); here $\lambda_0$ is the free air radiation wavelength, $n_2$ and $h_2$ are the refractive index and thickness, respectively, of layer 2, and $\theta_2$ is the refraction angle. The model can be extended to more layers by recursively defining $R_{23}$ as $R_{234}$, using Eq. (1), where 4 denotes the fourth layer. In our case, for example, the layers were air–epitaxy–substrate–air. However, the third layer was optically dense (a highly doped substrate), allowing us to neglect reflections from its back surface. The reflection coefficients were taken for parallel-
polarized radiation. Their dependence on the doping densities of the semiconductor layers is given (through the dielectric function) by the Drude model:

\[
e(\omega) = \varepsilon_\infty \left( 1 - \frac{\omega_p^2}{\omega^2 + i\omega/v} \right) \varepsilon_0,
\]

where \(\varepsilon_\infty\) is the dielectric coefficient at high frequencies, \(\varepsilon_0\) is the dielectric constant of vacuum, and \(\omega\) is the frequency of the electromagnetic waves. \(\omega_p\) and \(v\), the plasma and collision frequencies, are defined by

\[
\omega_p^2 \frac{n e^2}{\varepsilon_0 m_{\text{eff}}}
\]

and

\[
v = \varepsilon_0 \omega_p^2 \rho_{\text{DC}},
\]

where \(n\) is the doping density, \(\rho_{\text{DC}}\) is the resistivity at \(\omega \to 0\), and \(m_{\text{eff}}\) is the effective mass of the electrons (or holes) in the doped layers. In order to find the dc resistivity we use \(\rho_{\text{DC}} = 1/e n \mu\) and the empirical relation between the electron/hole mobility and the doping density, which states

\[
\mu = \mu_{\text{min}} + \frac{\mu_{\text{max}} - \mu_{\text{min}}}{1 + \left(\frac{n}{n_0}\right)^\alpha},
\]

where \(\mu_{\text{min}}, \mu_{\text{max}}, n_0\), and \(\alpha\) are constants dependent on the type of doping ions.

III. EXPERIMENTAL SETUP

The THz pulses are created by focusing a 100 fs mode-locked Ti:sapphire laser, with a repetition rate of 82 MHz and an average power of 40 mW, on the positive electrode of a gold-on-GaAs coplanar transmission line biased at 50 V. This radiation generation effect was investigated and described by Fattinger et al., and is being used almost as a standard source for THz radiation. Using THz optics consisting of a pair of aluminum parabolic mirrors and a set of two silicon lenses a parallel beam is generated and sent to a sample as shown in Fig. 1. The reflected THz beam is then directed through a symmetrical path and focused on a detector creating a small voltage drop across its dipole antenna. The detection of that voltage is done by focusing a time-delayed beam of the same laser on the gap at the center of a 30 \(\mu\)m dipole antenna embedded in an aluminum transmission line on a silicon-on-sapphire substrate. At the sample the THz pulse is polarized parallel to the incidence plane and its incidence angle is set to be \(\sim 20^\circ\). The reference is measured by replacing the sample with an aluminum mirror considered to be a 100% reflector. Special attention was paid to the device holding the samples and mirror in order to place their front surfaces with an accuracy of \(\sim 1\) \(\mu\)m.

IV. EXPERIMENTAL RESULTS AND DISCUSSION

The samples presented here are: (1) \(\sim 30\) \(\mu\)m thick \(n\) type epitaxy layer on a 600 \(\mu\)m thick, 3 in. in diameter, \(n^+\)
The amplitude spectrum of a THz pulse reflected from the n type sample, calculated by fast Fourier transform, is shown; the same size and a doping density of n = 3.6×10^{18} \text{ cm}^{-3}.

The amplitude spectrum of a THz pulse reflected from the n type sample, calculated by fast Fourier transform, is shown in Fig. 2(a) (solid line) in comparison to the reference amplitude spectrum (dotted line). The sharp feature at 0.55 THz is due to absorption by water vapor in the experiment enclosure. This can be eliminated by purging the enclosure with dry nitrogen, but has proved to be inessential to the experiment. The time-resolved measurements are shown in the inset. Figures 2(b) and 2(c) show the calculated (solid line) and measured (circles) amplitude ratios and relative phases of the Fourier transforms of the sample and reference. The sharp minimum in the reflection function around 0.7 THz caused by the interference between the reflections from the front and back surfaces of the epitaxy layer is clearly seen. Using Eqs. (2)–(4) and the dependence of the complex reflection coefficient on the dielectric function, the epitaxy layer doping density and thickness (n = 1.5×10^{15} \text{ cm}^{-3} and d = 28 \mu m) that best fit the data are found. We used a simple least-sum-of-squares method in a two-dimensional grid of the thickness and doping density of the layer. The doping density of the substrate was known and was introduced as a parameter to the computer program. In the calculations we allowed for a small freedom in the relative position of the sample (up to ± 1 \mu m). Only by fine tuning this value could we reach very accurate fits to the data. From the doping density both the frequency dependent and dc conductivity (or resistivity) can be calculated using

$$\sigma = \frac{i\varepsilon_0 \omega^2}{\omega + i\nu}.\quad (5)$$

In Fig. 3, we can see that the dc conductivity for the 30 \mu m sample is ~34/\Omega m, resulting in a resistivity of ~3 \Omega cm.

We have extended the data to 7 THz (omitting any other effects which might appear in these frequencies) to include the frequency of the crossing point of the real and imaginary parts of the conductivity, which is the collision frequency of the Drude model (see Ref. 1). The measurements and calculations of the 15 \mu m p type sample are shown in Fig. 4. For this sample a doping density n = 1.5×10^{16} \text{ cm}^{-3} and a thickness d = 15 \mu m were found to best fit our data (resulting in \rho_{DC} = 1 \Omega cm). Samples of varying thickness (15–58 \mu m) and resistivity (0.5–3 \Omega cm) were tested. The errors in our thickness calculations were all under 0.25 \mu m relative to the known value. The resistivity measurements all agreed within 5% with the resistivity measured by standard probes such as a capacitance–voltage probe and a four-point probe, except for the 15 \mu m sample, which had an accuracy of ~20%. Duvillaret et al.\textsuperscript{11} reach accuracies of 2% in the refractive index and 1% in the thickness of a 368 \mu m sample. Although our samples are significantly thinner, the sharp feature in the reflection function (in the 30 \mu m sample), as well as the
rapid change in the relative phase around 0.7 THz, helps calculate the thickness of the layer very accurately. In the 15 μm sample, where the sharp feature is beyond the range of good signal-to-noise ratio, the results are substantially less accurate. An additional difference is the way we incorporate the thickness into our calculations; in Ref. 9 the thickness is determined by minimizing the oscillations in the resulting refractive index.

V. CONCLUSION

We have shown the characterization of thin epitaxy layers using THz reflection spectroscopy. The doping density, thickness, and resistivity have been calculated using the Drude model. This technique can be extended to thinner layers. However, in order to achieve good accuracy broader band THz pulses12,13 must be used so that the sharp interference features of the reflection function, now appearing at higher frequencies, are detectable. We estimate that reaching layers of ~1 μm requires detecting frequencies of more than 20 THz.