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Temperature Dependence of Low Energy Carrier Dynamics of Silicon by Terahertz Time Domain Spectroscopy

Shigeki Nashima, Osamu Morikawa, Kazue Takata, Masanori Hangyo,

Abstract – **The complex conductivity of moderately P-doped silicon wafers (1.1±0.2 Ωcm) at various temperatures has been deduced by using a terahertz time-domain (THz-TDS) spectroscopy. The characteristic dispersion of the complex conductivity is observed in the THz region. Temperature dependence of the complex conductivity changes dramatically around ~120 K, which is interpreted in terms of enhancement of mobility and the freezing of the carrier. The experimental data at low temperatures slightly deviates from the simple Drude model, which causes the underestimation of the mobility and overestimation of the carrier density.**

I. INTRODUCTION

It is well known that the optical properties of semiconductors from microwave to infrared regions are greatly influenced by the dynamics of free carriers of semiconductors[1]-[6]. Dispersion of the complex conductivity (σ_1-$i\sigma_2$) depends on the carrier density and scattering time, which is explained by the simple Drude model. Such a model conversely provides a simple method of calculating optical constants in the far infrared region from the carrier density and mobility. However, the optical properties in this region at low temperatures have not been discussed so much before. The terahertz time-domain spectroscopy (THz-TDS) is used to measure the complex conductivity of samples at THz frequencies without the need of the Kramers-Kronig transformation[6]. In this letter, the complex conductivity of a moderately doped silicon wafer is deduced at various temperatures by using the THz-TDS. We obtain the carrier density and mobility of the sample at low temperatures and compare them with the results obtained from the Hall measurement and four-point contact resistivity.

II. EXPERIMENTAL

An *n*-type silicon wafer doped with phosphorus was used as a sample in this study. The resistivity at room temperature and the thickness of the sample were 1.1(±0.2) Ωcm and 400 μm, respectively. A conventional THz-TDS system was used wherein the pump and the trigger beams were derived from a mode-locked Ti:sapphire laser which produces optical pulses with a width of 50 fs and a wavelength of 790 nm at a repetition a rate of 82 MHz[4][5]. The sample was mounted on a sample holder of a closed-cycle He refrigerator specially designed to avoid mechanical vibrations and was inserted between a set of paraboloidal mirrors. In this measurement, a 5-μm gap bowtie-type photoconductive antenna was used as a THz emitter and detector. The frequency range of this system was limited by the absorption property of a 3-mm-thick fused quartz windows of the He refrigerator and was estimated to be less than 1.5 THz.

III. RESULTS AND DISCUSSION

We calculate the complex refractive index $\tilde{n}$ from experimental transmittance and phase shift obtained by the Fourier transformation of the THz pulse waveforms before and after inserting the sample. The complex conductivity is obtained from the complex refractive index from the relation,

$$\tilde{n}^2 = \tilde{\varepsilon}(\omega) = \varepsilon_{Si} + i\tilde{\sigma}(\omega)/\omega\varepsilon_0, \qquad (1)$$

where $\tilde{\varepsilon}(\varepsilon_1 - i\varepsilon_2)$ is the complex dielectric constant, ε_{Si} is the dielectric constant of undoped silicon and ε_0 is the free-space permittivity. We used the expression $\varepsilon_{Si}=(3.415)^2$[1]. Frequency dependence of the complex conductivity of the sample at 300 K, 120 K, 70 K, and 16 K is shown in Figs. 2(a)-(d), respectively. At room temperature the value of σ_1 decreases monotonically with increasing frequency. The value of σ_2 at room temperature increases from zero with increasing frequency until ~0.6 THz and decreases monotonically with increasing frequency further. At 0.6 THz, a crossover of the two curves is observed. Frequency dependence of the complex conductivity becomes pronounced with decreasing temperature until ~120 K. The value of σ_1 in the low frequency region increases and that in the high frequency region decreases with decreasing temperature. The temperature dependence of σ_2 also becomes pronounced with decreasing temperature. The crossover point of the two curves shifts to the lower frequency region with decreasing temperature. The dispersion of the complex conductivity decreases rapidly with decreasing temperature below 120 K and the values of σ_1 and σ_2 at 16 K are almost zero over the entire frequency region.

S. Nashima, O. Morikawa, K. Takata, M. Hangyo are with Reserch Center for Superconductor Photonics, Osaka University, 2-1 Yamadaoka, Suita, Osaka 565-0871, Japan

Solid lines in Fig. 1 show the fitting curves to σ_1 and σ_2 at each temperature using the simple Drude model. According to the simple Drude model, in which the collision damping is independent of the carrier energy, the frequency-dependent complex conductivity in SI units is given by

$$\tilde{\sigma} = i\varepsilon_0\omega_{\mathrm{p}}^2/(\omega + i\Gamma)\ , \qquad (2)$$

where $\Gamma=1/\tau$ is the carrier damping rate and τ is the average collision time. The plasma frequency ω_{p} is defined by $\omega_{\mathrm{p}}^2=N_{\mathrm{c}}e^2/\varepsilon_0 m^*$, where N_{c} is the number density of carriers, e is the electronic charge and m^* is the effective carrier mass. The expression $m^*=0.26\ m_0$ is also used, where m_0 is the free-electron mass[7]. Our fitting procedure effectively optimizes the values of N_{c} and τ, from which the mobility μ given by $\mu=e\tau/m^*$ is determined. The two parameters are determined by fitting the complex conductivity data between 0.2 and 1 THz.

Figure 2 (a) shows the temperature dependence of the mobility obtained from the fitting (open circles). Solid and dashed lines show the data obtained from previous Hall measurements on two samples with smaller and larger resistivities ($\rho=0.66$ Ωcm, 4.76 Ωcm) than the present sample, respectively[8]. Error bars show the uncertainties associated with temperature. At room temperature the value of μ and ρ (=$1/\sigma(0)$) is estimated to be 1560 cm^2/Vs and 1.06 Ωcm for the present sample, respectively, which agree on the whole with that obtained by Hall measurement and four-point contact resistivity measurement[9]. The value of μ increases dramatically with decreasing temperature until 150 K. The increasing rate gradually decreases with decreasing temperature. However, the value of μ obtained by the simple Drude fit at various temperatures is a little smaller than that of the silicon with lower resistivity obtained from the Hall measurement.

Figure 2 (b) displays the temperature dependence of the carrier density (open circles) of the sample obtained from the simple Drude fit. According to the Fermi-Dirac distribution, the carrier density of moderately doped silicon at various temperatures satisfies the following equation,

$$\frac{N_{\mathrm{c}}{}^2}{N_{\mathrm{D}} - N_{\mathrm{c}}} = N_\upsilon \cdot \left(\frac{2\pi\, m_{\mathrm{n}} k_{\mathrm{B}} T}{h^2}\right)^{3/2} \exp\left(-\frac{\Delta E_{\mathrm{D}}}{k_{\mathrm{B}} T}\right), \qquad (3)$$

where N_{D} is the donor density, N_υ is the number of the valley at the X point, m_{n} is the effective mass, k_{B} is the Boltzman constant, T is the temperature, h is the Planck constant, and ΔE_{D} is the donor ionization energy of the phosphorus dopant. The value of N_υ is 6. The values, $N_{\mathrm{D}}=3.4\mathrm{x}10^{15}$ cm^{-3} (solid lines) and $5\mathrm{x}10^{15}$ cm^{-3} (dashed lines), are used corresponding to $\rho=1.1+0.2$ Ωcm and 1.1-0.2 Ωcm (the positional fluctuation of the resistivity of the present sample)[10]. The expression $m_{\mathrm{n}}=(m_{\mathrm{t}}{}^2 m_{\mathrm{l}})^{1/3}=0.32m_0$ is also used, where m_{t} and m_{l} are longitudinal and transverse masses at the X point, respectively. At room temperature, the experimentally

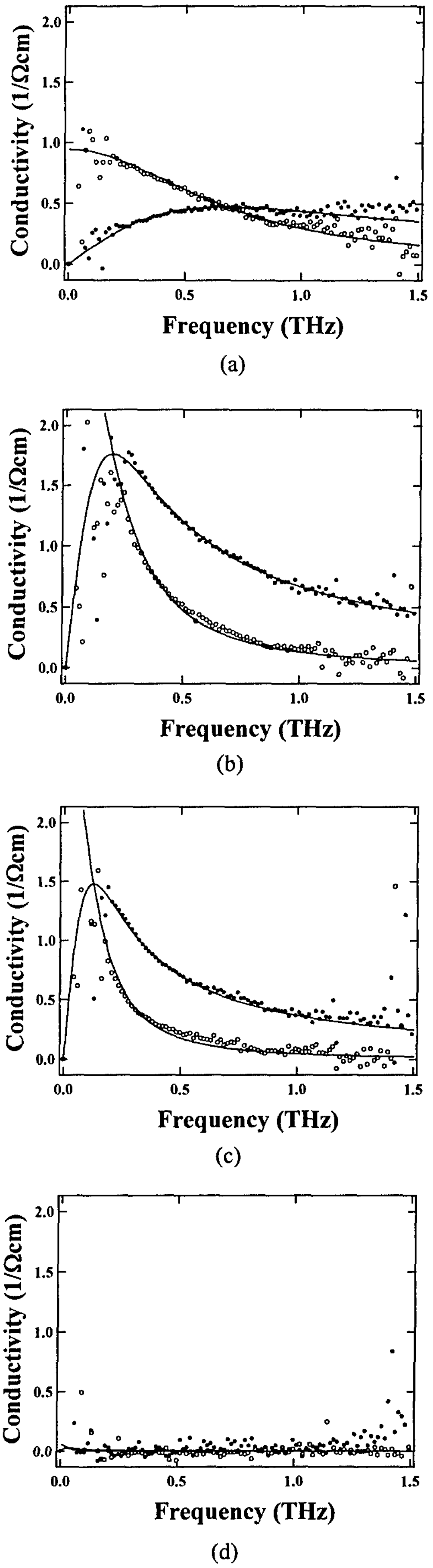

Fig. 1. Temperature dependence of the complex conductivity σ_1 (open circles) and σ_2 (solid circles) at (a) 300 K, (b) 120 K, (c) 70 K, and (d) 16 K. Solid lines show the simple Drude model.

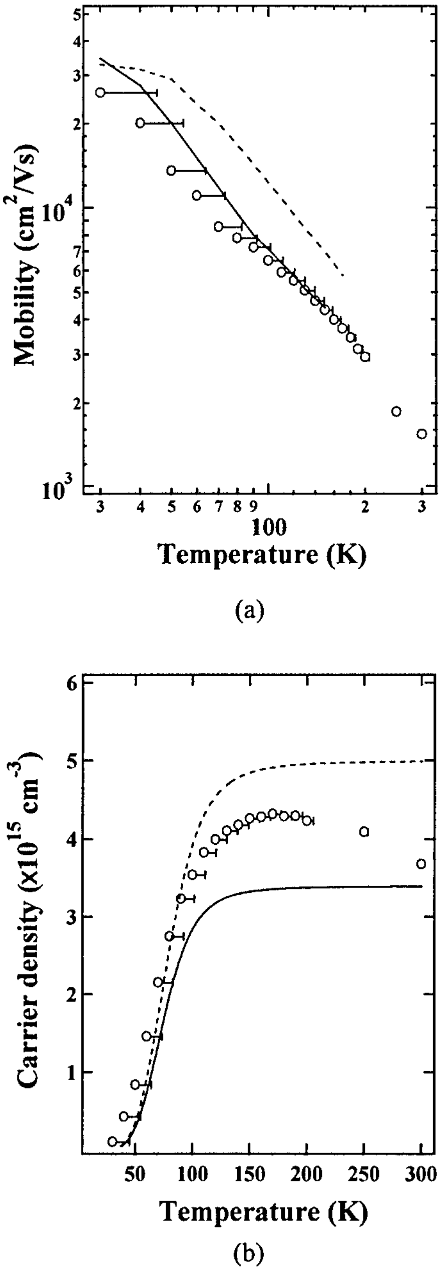

Fig. 2. Temperature dependence of (a) mobility and (b) carrier density deduced from the simple Drude fit to the complex conductivity obtained from the THz-TDS measurement. The solid and dashed lines in (a) show the results from Hall measurements for silicon with resistivity of 0.66 Ωcm and 4.76 Ωcm, respectively. The solid and dashed lines in (b) show the carrier density calculated using Eq. (3) assuming N_D=3.4x10^{15} cm^{-3} and 5x10^{15} cm^{-3} as a function of temperature, respectively.

obtained N_c is found to be 3.7x10^{15} cm^{-3} for the present sample. The experimentally obtained value of N_c increases slightly with decreasing temperature until 150 K and rapidly drops to zero. Below 30 K, the accurate estimation of the carrier density from the experimental results is difficult because of small frequency dependence of complex conductivity compared to the noise level.

At room temperature, the results obtained from THz-TDS agree well with the simple Drude model. However, the deviation from the simple Drude model is observed at low temperatures as shown in Figs. 1(a)-(d). The value of σ_1 at low frequency region obtained from THz-TDS is smaller than that obtained from the simple Drude model, which is similar to the results reported by Exter *et al*[4]. Deviation from the simple Drude model becomes more pronounced with decreasing temperature. We calculate $\mu(\omega)$ and $N_c(\omega)$ from the experimental complex dielectric constant at each frequency at various temperatures by the following equations[2].

$$\mu(\omega)=\frac{e}{m^*}\frac{\varepsilon_\infty-\varepsilon_1}{\omega\varepsilon_2}, \qquad (4)$$

$$N_c(\omega)=\frac{m^*\omega}{e^2\tau}\left\{\varepsilon_0\varepsilon_2\left(1+\omega^2\tau^2\right)\right\}, \qquad (5)$$

The dispersion of $\mu(\omega)$ and $N_c(\omega)$ at various temperatures are plotted in Figs. 3 (a) and (b), respectively. At room temperature, the value of $\mu(\omega)$ is constant over the entire frequency region, which indicates that the experimental results agree well with the simple Drude model. However, the values of $\mu(\omega)$ at low temperatures decrease with increasing frequency, which means disagreement with the simple Drude model. This dispersion is also observed at 90 K in the millimeter wave region and is explained by the calculation based on the Boltzman transport equation[3]. The dispersion of $\mu(\omega)$ becomes more

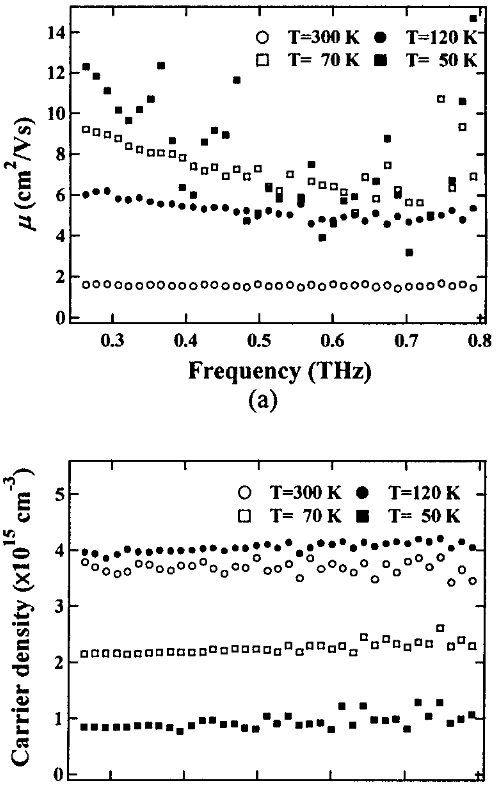

Fig. 3. The dispersion of (a) μ and (b) N_c obtained from the experimental dispersion of ε_1 and ε_2 at 300 K (open circles), 120 K (solid circles), 70K (open squares), and 16 K (solid squares).

pronounced with decreasing temperature. Below 50 K $\mu(\omega)$ is difficult to estimate because of small frequency dependence compared to the noise level. These results indicate that $\mu(\omega = 0)$ is larger than μ obtained from the simple Drude fitting in the entire frequency region. Although the value of $N_c(\omega)$ at room temperature is also constant as well as $\mu(\omega)$, the change of $N_c(\omega)$ with frequency is observed at low temperatures. The value of $N_c(\omega)$ slightly increases with increasing frequency, which predicts that N_c at low temperatures obtained from the simple Drude model estimates a slightly larger than that obtained from $N_c(\omega = 0)$.

IV. CONCLUSION

The THz-TDS system is used to measure the complex conductivity of *n*-type silicon wafer at temperatures from 16 K to room temperature. The measured complex conductivity is well fitted by the simple Drude model at room temperature and the experimentally obtained carrier density and mobility agree on the whole with Hall measurement and four-point contact resistivity. This result indicates that the THz-TDS measurement is an effective method for electric noncontact characterization of doped silicon. The change of the temperature dependence of the complex conductivity around ~120 K is observed and slight deviation from the simple Drude model is found at low temperatures. This deviation causes the calculation of the mobility and carrier density using the simple Drude model in the entire frequency region to be slightly underestimated and overestimated, respectively.

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