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Analysis of the Transient Photoconduction of β-Rhombohedral Boron, Allowing the Carrier Injection from Electrode

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The transient photoconduction of β-rhombohedral boron was analyzed within the framework of the band theory. Since the dielectric relaxation time was shorter than observed time, the longitudinal photocurrent was analyzed on the condition that the carrier injection from the irradiated electrode was allowed. The hole mobility at room temperature estimated by way of best fit on the assumption of one kind of trap was 6 $cm^2/V \cdot s$ and 7 $cm^2/V \cdot s$ for samples made by Niemyski and Wacker Chemie, respectively. © 1997 Academic Press

INTRODUCTION

We investigated the transient longitudinal photoconduction of β-rhombohedral boron to get the mobility of mobile holes free from the effect of traps. In the previous reports (1), we took account of the inhomogeneous electric field due to space charge of trapped holes and also made measurements on a sample with an oxide layer under the irradiated electrode to reduce the carrier injection. However, we could not obtain remarkable improvement although the results were favorable to the polaron model (2) of transport properties. In this report, we simulate the transient photocurrent in the framework of the band theory and try to calculate the transient photocurrent allowing the carrier injection from irradiated electrode. The carrier injection was neglected in the theory of trap-controlled transient photoconduction given by Schmidlin (3), which was the basis of our analysis in the previous reports.

EXPERIMENTAL

The experimental results on two samples were simulated. The one was made by Prof. T. Niemyski in Poland and the other was made by the Wacker Chemie Co. in Germany. The data on the Polish-made sample were the same as those in the previous report (1). The data on the German-made sample were new, but they were obtained by the same system. The dimension of the sample was about $5 \times 3 \times 1$ mm^3 and gold electrodes were made by sputtering. The side of a mesh-type electrode was irradiated by a ruby laser. The wavelength of the light pulse was about 6940 Å, which is a little shorter than the absorption edge of β-rhombohedral boron. The measurements were carried out from room temperature to about 100°C.

In our measurement, a dc voltage was applied to the sample at first, and the dark current was balanced out by means of the bridge circuit. The out-of-balance voltage was measured as the response of the longitudinal photocurrent after the irradiation of the mesh-type electrode by a ruby laser. The electric field was parallel to the light beam and only holes of the photocarriers were driven to the opposite electrode. Since the dielectric relaxation time of our sample was about 10 μsec and the photocurrent was observed up to the order of second, the effect of carrier injection from the irradiated electrode could not be neglected.

METHOD OF SIMULATION

The simulation of photocurrent was carried out in two stages.

In the first stage, the mobility μ of carriers was assumed at a certain value. Then the trap density was calculated following the theory of the space charge limited current (4), the resistivity being set at the measured value. Then density of mobile holes at the boundary between the sample and the electrode was estimated by the diffusion theory of the current through the Schottky barrier (5).

In the calculation of the dark current, the sample was assumed to have only one kind of traps at an energy $E_t(x)$ with the homogeneous density, N_t, for simplicity. The top of the valence band lies at an energy $E_v(x)$ and the effective level density of the band is N_v. The density of the mobile holes and the trapped holes at x, at time t, are $p(x, t)$ and $p_t(x, t)$ respectively. The local electric field, $E(x)$, is given by the Poisson equation,

$$(\varepsilon/q)(dE(x)/dx) = p(x, 0) + p_t(x, 0) - M, \qquad [1]$$

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where ε is the static dielectric constant, q is the magnitude of the electronic charge, and M is the charge density, $p + p_t$, at a position of no local field. In this stage only the dark current J_d was assumed to flow at $t = 0$. When the diffusive part of the current is neglected, a current flow equation is given by

$$J_d = q\mu p(x, 0) E(x) = \text{constant}. \quad [2]$$

It was also assumed that $p(x, 0)$ and $p_t(x, 0)$ were in quasi-thermal equilibrium. When the origin of the energy was taken at $E_v(0) = 0$, they were connected by

$$p_t(x, 0) = N_t[1 + \{N_v - p(x, 0))/p(x, 0)\} \exp\{-E_{t0}/k_B T\}]^{-1}, \quad [3]$$

where $E_{t0} = E_t(0)$, is the energy difference between the hole trap and the top of the valence band. As one of the boundary conditions on the Poisson equation, $p(0,0)$ was determined following the diffusion theory of the current through the Schottky barrier given by Mott (5). The density $p(0, 0)$ of mobile holes in the boron sample at the boundary will be determined by the same Fermi distribution function as for the electrons in the gold metal electrode. Thus $p(0,0)$ is given by

$$p(0, 0) = \int_0^\infty N(E)dE[1 + \exp\{(E - \phi + \chi)/k_B T\}]^{-1},$$

where $N(E)$ is the density of states in the sample, ϕ is the work function of the metal, χ is the electron affinity of the sample, k_B is the Boltzmann constant, and T is the absolute temperature. Usually $\phi - \chi \gg k_B T$, so that $p(0, 0)$ can be given approximately by

$$p(0,0) = N_v \exp\{-(\phi - \chi)/k_B T\} = N_v \exp\{-D_w/k_B T\},$$

where the effective level density is given by

$$N_v = 2\{2\pi m^* k_B T/h^2\}^{3/2},$$

and

$$D_w = \phi - \chi,$$

where m^* is the effective mass of mobile holes and h is Planck constant. As for the other boundary conditions, $p_t(0, 0)$ is calculated by Eq. [3] and $E(0)$ is given by Eq. [2] from $p(0, 0)$ and J_d.

In the calculation, $\varepsilon = 10.0\varepsilon_0$, $E_{t0} = 0.23$ eV, and $m^* = 2.0\, m_0$, where m_0 is the electron mass, were adopted according to the data shown in the Landolt–Boernstein table (6). The dark current at the lowest applied voltage was calculated from a measured value of resistivity and N_t, M, and D_w were treated as parameters.

When the mobility was assumed at a certain value, the parameters were determined to give the lowest applied voltage and $E(x)$, $p(x, 0)$, and $p_t(x, 0)$ could be obtained. In the case of higher applied voltage, N_t and M were fixed at the values obtained at the lowest voltage, and only D_w was changed as a parameter to get the applied voltage, because the Ohmic law is not satisfied by the space charge limited current.

In the second stage, the mobility, the release and the capture rate of holes were calculated following rate equation used by Schmidlin (3), without an assumption of homogeneous electric field, the photocurrent being fitted to the measured values.

At a point x, where holes are captured by and released from traps, the appropriate continuity equations are given by

$$\partial p/\partial t = \eta\, \delta(x)\, \delta(t) + r\, p_t(N_v - p) - (w/\mu E(x)) p(N_t - p_t) - (\partial f_p/\partial x), \quad [4]$$

$$\partial p_t/\partial t = (w/\mu E(x)) p(N_t - p_t) - r\, p_t(N_v - p), \quad [5]$$

$$f_p(x, t) = p(x, t)\, \mu E(x), \quad [6]$$

where η is the rate of hole generation at the surface by the irradiation of light pulse, r and w are the release and capture rates of the traps, and $f_p(x, t)$ is the flux of mobile holes. In this stage, N_t and $E(x)$ were fixed at the values obtained in the first stage. The initial values of $p(x, 0)$ and $p_t(x, 0)$ were those obtained in the first stage. The calculated photocurrents were fitted to measured values in the case of two applied voltages simultaneously, as r, w, μ and the scale factors of photocurrent were treated as parameters.

In order to allow the carrier injection from the irradiated electrode, the density of mobile holes and trapped holes at the boundary, that is, in the first pixel along x, were fixed at the values obtained in the first stage, which are in thermal equilibrium with the gold electrode. Then the photocarriers were generated at the second pixel at $t = 0$, in the process of solving the continuity equations.

A kind of iteration was performed until the difference between the mobility assumed in the first stage and that obtained in the second stage, became less than 1%. At present the simulation was successful only on the data obtained at room temperature. Therefore temperature dependence of the mobility could not be obtained.

RESULTS AND DISCUSSION

The simulation in the sense of convergence could not be carried out until now. One of the main reasons was that the

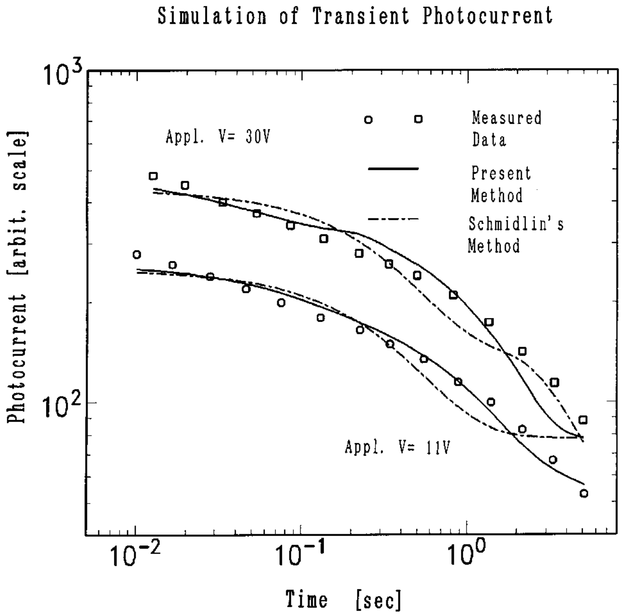

FIG. 1. The results of the simulation at a consistent value of mobility, 6 $cm^2/V \cdot s$, on a Polish-made sample, allowing the carrier injection from the irradiated electrode. The results of the simulation, following the theory of Schmidlin on a model with one kind of trap, were also shown. The value of mobility obtained in this case was 1.5×10^{-4} $cm^2/V \cdot s$.

unique solution could not be obtained in the first stage. In order to obtain a consistent value of mobility, the iteration between first and the second stages could also be made only by means of trial and error. Therefore our present results may be a kind of example. A consistent value of the mobility was obtained near 6 $cm^2/V \cdot s$, where N_t was 1.6×10^{19} cm^{-3}, on the Polish-made sample. The results of simulation is shown in Fig. 1. The degree of simulation is worse than that in the previous reports. In one of the previous reports when the homogeneous electric field was assumed, as in the paper by Schmidlin (3), a model with two kinds of traps was adopted to improve the simulation. To compare with the present results, the simulation of previous type was carried out on a model with one kind of trap and the homogeneous field, where the estimated mobility was 1.5×10^{-4} $cm^2/V \cdot s$. This results are also shown in Fig. 1. The degree of simulation was worse than in the present result. The same simulation on the German-made sample was performed, but the degree of simulation was much worse than in the case of the Polish-made sample. The estimated mobility was 7 $cm^2/V \cdot s$.

The transverse photoconduction of β-rhombohedral boron has been investigated by Nadolny (7). In this case photogenerated electrons can also flow through a sample, so that recombination process could be more complicated than in our longitudinal photoconduction. The same longitudinal photoconduction was investigated by Takeda (8) by means of inserting a layer of insulator between irradiated electrode and bulk boron to block carrier injection. A dc voltage was applied at the same time as irradiation through the blocking layer, so that the accelerating field acting on carriers would depend on the time constant of circuit, but they analyzed with a constant field.

Nadolny (7) found two kinds of carrier traps and Werheit (9) suggested six electron traps. However, only one carrier trap was introduced in this paper, because the calculation of space charge limited current was not easy in the case of two traps.

Although the simulation could not be made in the sense of convergence, a method of taking account of the carrier injection is proposed and the magnitude of mobility seems to depend much on the process of simulation.

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