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Characterization of deep centers in semi-insulating SiC and HgI$_2$: Application of discharge current transient spectroscopy

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Abstract In order to characterize traps in semi-insulating 4H-SiC and HgI$_2$ regarded as an attractive semiconductor for X-ray detectors, we apply discharge current transient spectroscopy (DCTS), which is a graphical peak analysis method based on the transient reverse current of a diode. In high-purity semi-insulating 4H-SiC whose diode may detect X-rays or γ-rays, DCTS can detect two types of trap species, and can determine those densities and emission rates. The emission rates of detected traps are close each other, suggesting that thermally stimulated current (TSC) may not distinguish between these two types of traps. In semi-insulating HgI$_2$, the densities and emission rates of two types of trap species are also determined by DCTS. Therefore, it is demonstrated that DCTS is a powerful method for determining the densities and emission rates of traps in semi-insulating semiconductors.

1. Introduction

High-purity Si pin diodes, Li-doped Si Schottky barrier diodes, and high-purity Ge pin diode have been developed for use in X-ray energy spectroscopy. In order to form a wide depletion region in a diode, a high reverse bias (e.g., -100 V) is applied to the diode. Since the resistivities of high-purity Si and Ge are not high enough to reduce the reverse current of the diode at room temperature to 1 nA, highly resistive HgI$_2$ and CdTe have been investigated. However, deep defects such as generation centers in semiconductors degrade the performance of X-ray detectors. When the high reverse bias is suddenly applied from 0 V, moreover, a transient reverse current due to these defects flows, which breaks a junction field-effect transistor connected to the detector by DC coupling. Recently, SiC has been highly purified, and its resistivity is much higher than 10^6 Ωcm. Compared with V-doped semi-insulating 4H-SiC, deep defects in high-purity semi-insulating 4H-SiC are considered to be much lower. In order to determine a possibility of high-purity SiC being used as a portable X-ray detector operating at room temperature, therefore, it is necessary to investigate deep defects in the semi-insulating semiconductor.

There are transient capacitance methods for determining the densities and energy levels of defects (i.e., traps), for example, deep level transient spectroscopy [1] and isothermal capacitance transient spectroscopy [2] for low-resistivity semiconductors, and the heterojunction-monitored capacitance method [3] for high-resistivity semiconductors such as undoped hydrogenated amorphous silicon. In the case of applying the transient capacitance methods to metal-insulator-semiconductor diodes, traps at the insulator-semiconductor interface can mainly be investigated [4]. In a semi-insulating semiconductor diode, however, the measured capacitance is a capacitance determined by the thickness of the diode, not determined by the depletion region of the junction. This is because the dielectric relaxation time becomes large due to its high resistivity [3]. Therefore, it indicates that it is difficult to determine the densities and energy levels of traps in semi-insulating semiconductors and insulators by transient capacitance methods.

Thermally stimulated current (TSC) is suitable for evaluating the densities and emission rates of traps with one thermionic emission rate or with completely different thermionic emission rates in semi-insulating

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semiconductors and insulators [5]. However, it is difficult to fit a TSC simulation to the experimental TSC data in the case of the material including more than one type of trap with close emission rates. Moreover, since the influence of the pyroelectric currents and the temperature dependence of the steady-state leakage currents must be considered when the measurement temperature increases continuously, an isothermal measurement is more suitable for evaluating the densities and emission rates of traps than TSC.

Although the densities and emission rates of traps can be obtained by fitting a simulation to the experimental transient current at a constant temperature, one should assume the number of trap species before the curve-fitting procedure, indicating that the determined values of densities and emission rates strongly depend on the assumed number of trap species. Moreover, in the curve-fitting procedure, the too many curve-fitting parameters (i.e., densities and emission rates) should be changed simultaneously, suggesting that the obtained values should be less reliable.

Without any assumption of the number of trap species, on the other hand, one of the authors has proposed a graphical peak analysis method for determining the densities and emission rates using the isothermally measured transient current, referred to as discharge current transient spectroscopy (DCTS) [6-8], and has applied it to SiN_x films [6], $Pb(Zr,Ti)O_3$ films [7], and high-resistivity Si pin diodes [8]. From each peak of the DCTS signal, the density and emission rate of the corresponding trap can be determined accurately.

In this study, we report on our investigation of a possibility of DCTS determining traps in semi-insulating 4H-SiC and HgI_2.

2. Experiment

A 0.37 -mm-thick high-purity semi-insulating 4H-SiC wafer was purchased from Cree Inc. Ni with a radius of 1.25 mm (top electrode) was evaporated onto one side of the sample, and Ni (bottom electrode) was evaporated over the other side of the sample. A 0.53 -mm-thick semi-insulating HgI_2 wafer was obtained from Constellation Technology. A carbon electrode with 3×2.5 mm^2 (top electrode) was formed, and a carbon electrode (bottom electrode) was formed over the other side of the sample.

DCTS measurements were performed at a reverse bias (V_R) of -100 V at 373 K for the 4H-SiC, and 303 K for the HgI_2 using a Keithley 236 source-measure unit.

3. Discharge Current Transient Spectroscopy

Let us consider the transient reverse current $I_R(t)$ of a diode after V_R is suddenly applied from 0 V ($t = 0$ s). The $I_R(t)$ consists of two types of currents: (1) a steady-state reverse current (I_{SR}) and (2) a transient current $I_{TR}(t)$ that arises from the emission of charged carriers from traps. The total charge $Q(t)$ of trapped carriers in the diode decreases with t as

$$Q(t) = S \sum_i q N_{ti} \exp\left(-e_{ti} t\right), \tag{1}$$

where N_{ti} is the number of carriers captured at the i th trap per unit area at $t = 0$ s, e_{ti} is the emission rate of the i th trap, S is the junction area, and q is the magnitude of the electronic charge. Because the decrease of $Q(t)$ results in $I_{TR}(t)$,

$$I_{TR}(t) = -\frac{dQ(t)}{dt} = S \sum_i q N_{ti} e_{ti} \exp\left(-e_{ti} t\right). \tag{2}$$

In order to graphically determine N_{ti} and e_{ti} independently, we define a DCTS signal $D(t, e_{ref})$ as [7]

$$D(t, e_{ref}) \equiv \frac{t}{qS}\left[I_R(t) - I_{SR}\right] \exp\left(-e_{ref} t + 1\right), \tag{3}$$

which is theoretically expressed using Eq. (2) as

$$\begin{aligned} D(t, e_{ref}) &= \frac{t}{qS} I_{TR}(t) \exp\left(-e_{ref} t + 1\right) \\ &= \sum_i N_{ti} e_{ti} t \exp\left[-\left(e_{ti} + e_{ref}\right)t + 1\right] \end{aligned}, \tag{4}$$

where e_{ref} is the peak-shift parameter. The function of $N_{ti} e_{ti} t \exp\left[-\left(e_{ti} + e_{ref}\right)t + 1\right]$ has each peak at a peak time of $t_{peaki} = 1/(e_{ti} + e_{ref})$. From each peak of the DCTS signal, therefore, the values of N_{ti} and e_{ti} can be independently determined as follow:

$$e_{ti} = \frac{1}{t_{peaki}} - e_{ref} \tag{5}$$

and

$$N_{ti} = \frac{D\left(t_{peaki}, e_{ref}\right)}{1 - e_{ref} t_{peaki}}. \tag{6}$$

The WINDOWS application software for DCTS can be freely downloaded at our web site (http://www.osakac.ac.jp/labs/matsuura/).

4. Results and Discussion

4-1. High-purity semi-insulating 4H-SiC

The top electrode was biased, and the bottom electrode was grounded. Figure 1 shows the current-voltage ($I - V$) characteristics of the semi-insulating 4H-SiC diode at 373 K. Judging from the $I - V$ characteristics, this diode is considered to act as a back-to-back diode, indicating that both the Ni/4H-SiC contacts are Schottky barrier junctions (i.e., rectifying contacts). On the other hand, the difference between the magnitude of the currents at positive and

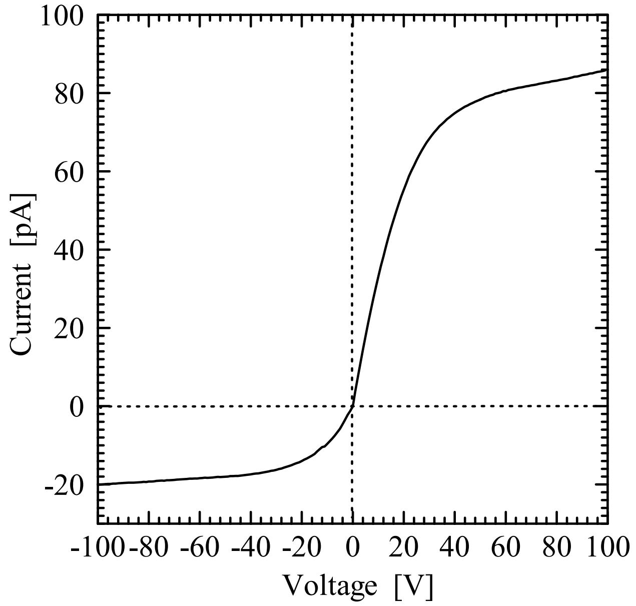

Fig. 1 Current-voltage characteristics for high-purity semi-insulating 4H-SiC diode

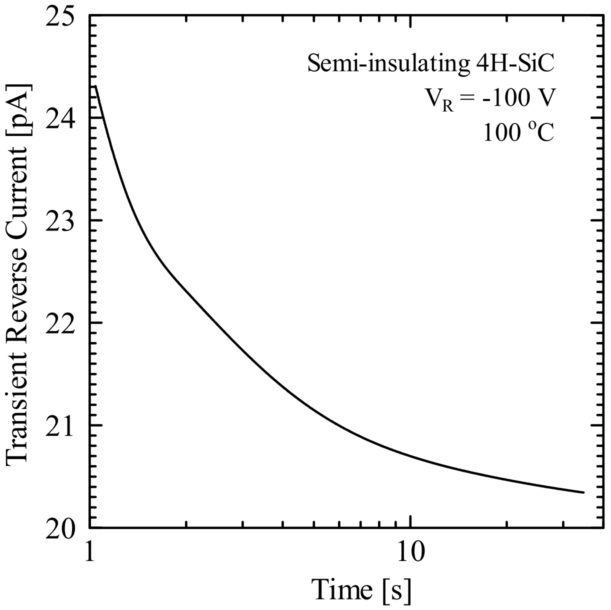

Fig. 2 Transient reverse current at -100 V at 373 K for semi-insulating high-purity 4H-SiC

negative biases is due to the difference in size between the electrodes. Therefore, at the negative bias the depletion region spreads from the top electrode to the bottom electrode because the reverse bias is applied to the top electrode, while at the positive bias it spreads from the bottom electrode to the top electrode.

Figure 2 shows $I_{\rm R}(t)$ at -100 V at 373 K in the semi-insulating 4H-SiC. Using the $I_{\rm R}(t)$, the DCTS signal with $e_{\rm ref} = 0\ {\rm s}^{-1}$ was calculated using Eq. (3), and is denoted by the solid line in Fig. 3. There is one peak, referred to as Max1 here. The time and value of Max1 are $3.2\ {\rm s}$ and $1.4\times10^{9}\ {\rm cm}^{-2}$, respectively, from which the emission rate ($e_{\rm t1}$) and sheet density ($N_{\rm t1}$) of the corresponding trap species (Trap1) were determined as $0.31\ {\rm s}^{-1}$ and $1.4\times10^{9}\ {\rm cm}^{-2}$, respectively, using Eqs. (5) and (6). When Trap1 is assumed to be uniformly distributed in the SiC, the density ($n_{\rm t1}$) of Trap1 is approximately $3.8\times10^{10}\ {\rm cm}^{-3}$.

The broken line in Fig. 3 is the DCTS signal with $e_{\rm ref} = -0.03\ {\rm s}^{-1}$. In the figure, another peak (Max2) appears, indicating that at least two types of trap species are included in the semi-insulating 4H-SiC. From Max2, the emission rate ($e_{\rm t2}$) and sheet density ($N_{\rm t2}$) of the corresponding trap species (Trap2) were determined as $0.10\ {\rm s}^{-1}$ and $1.2\times10^{9}\ {\rm cm}^{-2}$, respectively, using Eqs. (5) and (6). In the case that Trap2 is uniformly distributed in the bulk, the density ($n_{\rm t2}$) of Trap2 is approximately $3.2\times10^{10}\ {\rm cm}^{-3}$.

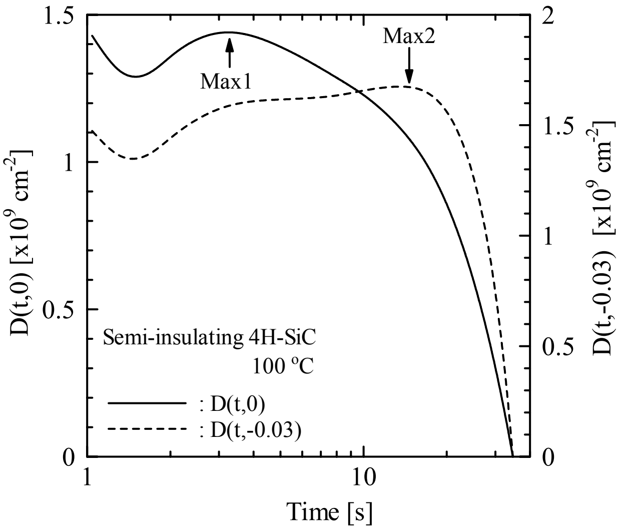

Fig. 3 DCTS signals with $e_{\rm ref}$ of 0 and -0.03 s^{-1}

In order to investigate other trap species and to determine whether the trap species determined above is a discrete trap or an energetically distributed trap, the value of $e_{\rm ref}$ changed. Figure 4 depicts the $e_{\rm ref}$ dependencies of the emission rate ($e_{\rm t}$) and sheet density ($N_{\rm t}$) determined from the maximum of $D(t, e_{\rm ref})$, denoted by the solid and broken line, respectively. Two discrete values of $e_{\rm t}$ or $N_{\rm t}$ clearly appear in the figure. Moreover, the $e_{\rm ref}$ range of the almost constant $N_{\rm t}$ clearly corresponds one to one to the $e_{\rm ref}$ range of the almost constant $e_{\rm t}$, indicating that two discrete trap species exist in this SiC, according to Ref. [7]. Therefore, it is found that DCTS can distinguish between two types of trap species (Trap1 and Trap2) with

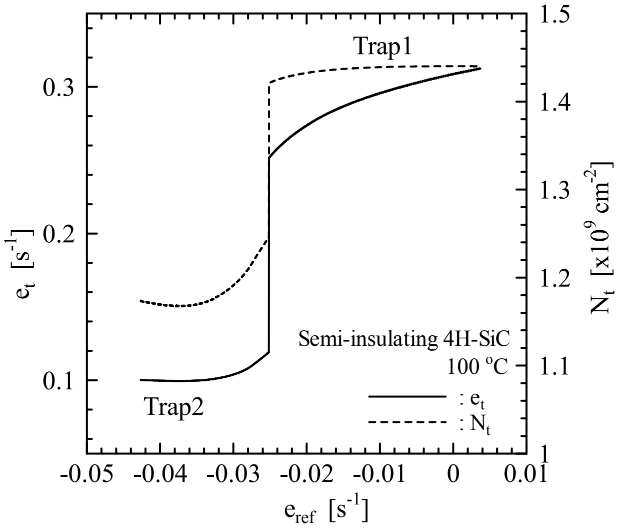

Fig. 4 e_{ref} dependence of e_{t} or N_{t} determined from maximum of $D(t, e_{\mathrm{ref}})$

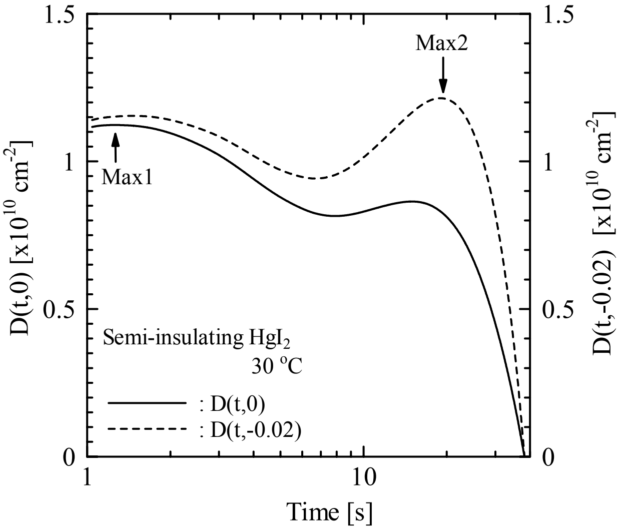

Fig. 6 DCTS signals with e_{ref} of 0 and -0.02 s^{-1}

close emission rates by changing e_{ref}.

4-2. Semi-insulating HgI$_2$

Figure 5 shows $I_{\mathrm{R}}(t)$ at -100 V at 303 K in the HgI$_2$. The DCTS signals with e_{ref} of 0 and -0.02 s^{-1} were calculated using Eq. (3), and are denoted by the solid and broken lines in Fig. 6, respectively. Figure 7 shows the e_{ref} dependence of e_{t} (the solid line) or N_{t} (the broken line) determined from the maximum of $D(t, e_{\mathrm{ref}})$. Two discrete values of e_{t} or N_{t} clearly appear in the figure. Moreover, the e_{ref} range of the almost constant N_{t} clearly corresponds one to one to the e_{ref} range of the almost constant e_{t}. Therefore, the emission rate and sheet density of one trap are approximately 0.78 s^{-1} and approximately 1.1×10^{10} cm^{-2}, respectively, while those of the other are approximately 0.072 s^{-1} and approximately 8.8×10^{9} cm^{-2}, respectively.

5. Conclusion

In order to precisely investigate electrically active traps in semi-insulating semiconductors, DCTS based on the transient current of a diode has been tested. In high-purity semi-insulating 4H-SiC, DCTS could

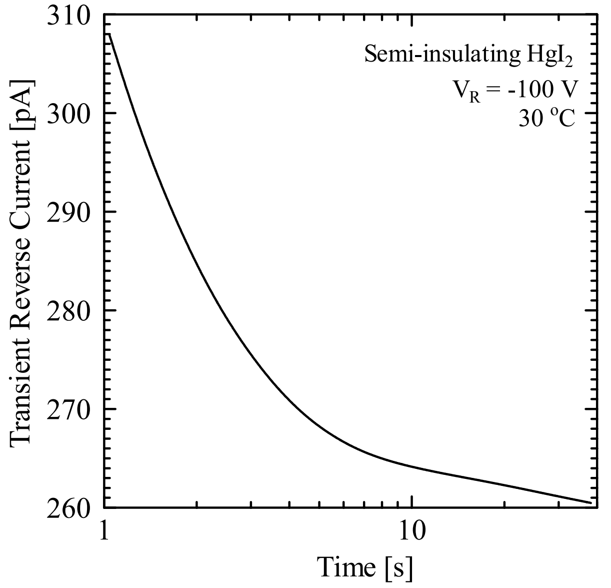

Fig. 5 Transient reverse current at -100 V at 303 K for semi-insulating HgI$_2$

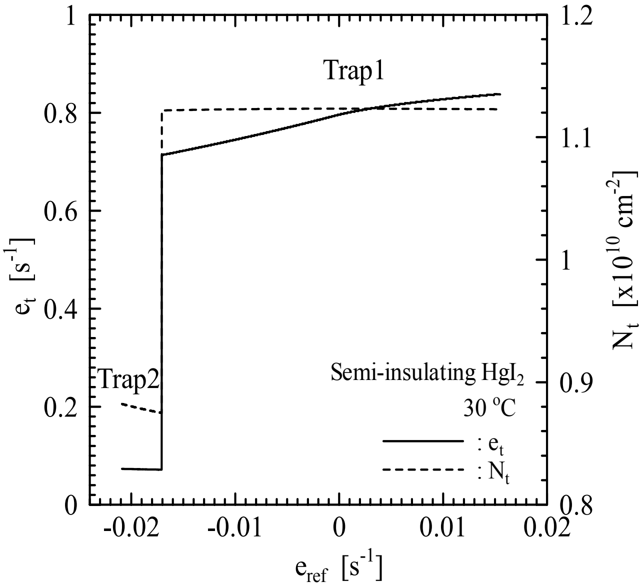

Fig. 7 e_{ref} dependence of e_{t} or N_{t} determined from maximum of $D(t, e_{\mathrm{ref}})$

distinguish between two discrete trap species with close emission rates of 0.1 and $0.3\ \mathrm{s}^{-1}$ at 373 K, and could also determine those densities. In semi-insulating HgI_2, the densities and emission rates of two types of trap species could be estimated. Therefore, it is demonstrated that DCTS is applicable to determining the densities and emission rates of traps in semi-insulating semiconductors, and is superior to TSC.

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