Influence of Nonuniform Microstructure of SiC Ceramic Semiconductor on Its Electrical Conductivity

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SiC セラミック半導体の微構造不均一性の電気伝導に及ぼす影響

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Several simulations were performed in order to estimate the effects of the nonuniformity of the SiC ceramic semiconductor microstructure on the electrical conductivity. The boundary potential model was used to express the electrical characteristics of the grain boundaries and the calculations were performed using the three-dimensional equivalent circuit in the simulations. These simulations show that the nonuniformity of the acceptor concentration or of the trap concentration at the grain boundary greatly affects the electrical conductivity of the SiC ceramic semiconductor. This is explained by the percolation theory. The influence of these nonuniformities should be carefully considered in order to design or to produce related devices.

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1. Introduction

SiC, a typical nonoxide ceramic, is a semiconductor which is stable at high temperatures, and it is expected to be used as a material for electronic devices such as the high-temperature thermistor¹⁾⁻⁴⁾ or the thermal battery.⁵⁾ The electrical properties of a ceramic semiconductor depend on the microstructure such as the grain size, the trap concentration at the grain boundary, the defects and the doping level in the grain.

It was already pointed out through rough calculations that such nonuniformity of the microstructure should be taken into account for the investigation of ceramic semiconductors.⁶⁾ Generally the size of the electronic devices tends to be reduced, and the effects of the nonuniformity appear clearly in the small devices. Thus more detailed investigation on the nonuniformity of the microstructure is required before SiC ceramics can be applied to the design and the production of related devices, especially small devices. However, it is difficult to investigate the effects of such nonuniformity experimentally because it is very hard to control the uniformity of microstructures in the sintering process.

In this study, the effects of nonuniformity on the electrical conductivity were estimated through simulations in which the acceptor concentration in the grain and the trap concentration in the grain boundary were considered as nonuniformities in the microstructure. It is pointed out that those nonuniform microstructures greatly influence the electrical conductivity of the SiC ceramic semiconductor, on the basis of the results of the simulations.

2. Models and theories

SiC ceramics are composed of SiC crystal grains and grain boundaries, as shown in Fig. 1(a), and each grain is considered to be a single-crystalline semiconductor. The grain boundary is the interface at which a grain comes into contact with another grain of different crystal orientation and at which dangling bonds exist.

Based on the results of related experiments,²⁾ two conditions were assumed in this simulation.

- (1) The conduction of the semiconductor is p-type.
- (2) The current flows in the grains and across the grain boundaries (I_{GB} in Fig. 1(a)), but does not flow along the grain boundaries ($I_G=0$ in Fig. 1(a)).

Under these assumptions, the grain boundary has positive charge, because the holes in each SiC grain are trapped

Fig. 1. Schematic models of the (a) microstructure, (b) charge distribution, (c) Schottky barrier and (d) equivalent circuit.

by the dangling bonds in the grain boundary. As a result, negative space charges are distributed in the grain near the grain boundary because negative ionized acceptors are left there. The number of trapped holes in a grain boundary is $N_T S$, where N_T is the trap concentration in the grain boundary and S is the area of the grain boundary between two grains. The number of ionized acceptors in a grain is expressed as $N_A W S$, where N_A is the effective acceptor concentration in the grain and W is the width of the space-charge layer. The number of holes, $N_T S$, is equal to the number of the acceptors, $N_A W S$, because the trapped holes in the grain boundary come from the acceptors in the grains on both sides, as shown in Fig. 1(b). Therefore the width of the space-charge layer is

$$W = \frac{N_T}{N_A} \quad (1)$$

An electric field is generated due to these space-charge distributions around the grain boundary, and then the Schottky barriers are formed on the both sides of the grain boundary, as shown in Fig. 1(c).

The barrier height Φ_B is calculated as follows. First, the electric field around the grain boundary is calculated based on the charge distribution. Using Poisson's equation,

$$\frac{d^2 \Phi_B}{dx^2} = \frac{e \cdot N_A}{\epsilon_0 \cdot \epsilon_S} \quad (0 < x \leq W/2), \quad (2)$$

where ϵ_0 is the dielectric constant in the vacuum and ϵ_S is the dielectric constant of SiC, for which the value of 10 is used here. Equation (2) is integrated and the electric field E is derived as

$$E = \frac{d\Phi_B}{dx} = \int_{W/2}^x \frac{e \cdot N_A}{\epsilon_0 \cdot \epsilon_S} dx = \frac{e \cdot N_A}{\epsilon_0 \cdot \epsilon_S} \left(x - \frac{W}{2} \right). \quad (3)$$

The barrier height Φ_B is obtained by integrating of Eq. (3).

$$\Phi_B = \int_{W/2}^0 \frac{e \cdot N_A}{\epsilon_0 \cdot \epsilon_S} \left(x - \frac{W}{2} \right) dx = \frac{e \cdot N_A}{2 \cdot \epsilon_0 \cdot \epsilon_S} \cdot \left(\frac{W}{2} \right)^2 \quad (4)$$

From Eq. (1) and Eq. (4), Φ_B can also be described by

$$\Phi_B = \frac{e \cdot N_T^2}{8 \cdot \epsilon_0 \epsilon_S N_A}. \quad (5)$$

The equivalent circuit of a grain boundary is shown in Fig. 1(d), where R_G is the resistance component in the grain, R_S is the resistance resulting from the Schottky barrier, and C_S is the capacitance around the grain boundary, which is expressed as

$$C_S = \frac{\epsilon_0 \epsilon_S S}{W} = \frac{\epsilon_0 \epsilon_S N_A}{N_T} \quad (6)$$

from Eq. (1). R_S is

$$R_S = R_0 \exp \left(\frac{e \Phi_B}{kT} \right), \quad (7)$$

where k is the Boltzmann constant. The admittance of the Schottky barrier Y_S is given as

$$Y_S = \frac{1}{R_S} + j2\pi f C_S, \quad (8)$$

where f is frequency.

3. Algorithm

In this simulation, the fluctuations of N_T and N_A were taken into account. N_T is the trap concentration in a grain boundary, and N_A is the acceptor concentration in a grain. The relationship between the parameters is shown in Fig. 2. N_T and N_A are determined so that $\log N_T$ and $\log N_A$ have normal distributions with the mean values of $\log N_{T0}$ and $\log N_{A0}$ and the standard deviations of S_T and S_A , respectively. Through the calculation procedure shown in Fig. 2, pairs of R_S and C_S are obtained, from which Y_S can be determined using Eq. (8).

These pairs of R_S and C_S are incorporated into the 3-dimensional circuit shown in Fig. 3. Each pair of R_S and C_S corresponds to a grain boundary. R_G in Fig. 1(d) is neglected because it is considered to be very small compared to R_S . The size of the sample was assumed to be $30 \mu\text{m}$ in width, $30 \mu\text{m}$ in length and $30 \mu\text{m}$ in height. Through a related experiment,⁷⁾ the average size of grains was found to be about $5 \mu\text{m}$. Therefore $5 \times 5 \times 5$ (5 in width, 5 in length and 5 in height) pairs of R_S and C_S were taken into account in the equivalent circuit shown in Fig. 3 for the calculation. Then Kirchhoff's law is used in order to obtain the current, which is converted to the electrical conductivity.

The flow chart of the simulation process is shown in

Fig. 2. Relationship between parameters used in simulation.

Fig. 3. Part of 3-dimensional equivalent circuit used for simulations. Each pair of R_S and C_S corresponds to a grain boundary. Pairs of $5 \times 5 \times 5$ (5 in width, 5 in length, 5 in height) were taken into account here.

Fig. 4. Flow chart for obtaining electrical conductivity σ of SiC ceramic semiconductor.

Fig. 4. A random number generator was used in order to determine N_T and N_A . f is the frequency of the current and T is the temperature.

4. Results and discussion

4.1 Frequency dependence of electrical conductivity

The frequency dependence of the calculated electrical conductivity is shown in Fig. 5. S_T is taken as a parameter and S_A is assumed to be zero here. The sample is assumed to have $5 \times 5 \times 5$ grain boundaries, as described in Section 3. Each line in Fig. 5 shows the average of the calculated electrical conductivity which corresponds to respective S_T . In the low-frequency (low- f) region, the frequency dependence is not observed. However, in the high-frequency (high- f) region, the electrical conductivity increases with

Fig. 5. Frequency dependence of electrical conductivity. Lines indicate calculated results. Calculations were done under the assumption that sample has $5 \times 5 \times 5$ grain boundaries. Plots show experimental results for a sample with 1.5 mm in thickness and 15 mm in diameter.

the increase of frequency. This frequency dependence is explained by Eq. (8) which indicates that the current tends to flow through R_S in the low- f region and through C_S in the high- f region in Fig. 1(d). When S_A is used as the parameter, a similar tendency was also observed.

The measured electrical conductivity of a sample which has 1.5 mm in thickness and 15 mm in diameter is also plotted in Fig. 5. For a sample of this size, the nonuniformity of the microstructure is considered to have little effect on the electrical conductivity which approaches the value when both S_T and S_A are zero ($S_T=0$ in Fig. 5) because there are many grain boundaries in a sample of this size and because their electrical characteristics are averaged over all the grain boundaries. The experimental and calculated values are in good agreement, which supports the validity of this simulation.

4.2 Variation of the electrical conductivity

As shown in Fig. 5, the increase of S_T tends to increase the average of the electrical conductivity in the low- f range. Figure 6 shows a histogram of calculated electrical conductivity for DC when S_T (Fig. 6(a)) and S_A (Fig. 6(b)) are taken as parameters. As shown in Fig. 6, the electrical conductivity tends to increase and its variation tends to be widened as S_T or S_A increases.

These results are explained by the percolation theory⁸⁾⁻¹⁰⁾ as follows. The variation of N_T or N_A causes the variation of R_S , as shown by Eq. (5) and Eq. (7). As a simplified model of the variation of R_S , we consider the circuit network shown in Fig. 7, where R_S is classified into two categories, high resistance (high R_S) and low resistance (low R_S). There exists the possibility that the current paths are formed only with the low R_S between the electrodes. Then the electrical conductivity increases because the cur-

(a)

(b)

Fig. 6. Histogram of calculated electrical conductivity for DC. S_T (a) and S_A (b) are taken as parameters.

Fig. 7. Simplified model of R_S variation. Resistors drawn in bold lines have low resistance (low- R_S) and those drawn in fine lines have high resistance (high- R_S). Four low- R_S resistors exist in both (a) and (b). Electrodes are (a) linked and (b) not linked by low- R_S resistors.

rent tends to flow only through paths like those shown in Fig. 7(a). This probability, which is called the percolation probability, depends on the ratio of the number of low- R_S resistors to the total number of resistors. With the increase of this ratio, the percolation probability increases. The actual situation is similar to this simplified case. The large S_T tends to cause a large variation of R_S , and many of the resistors have low resistance, which then tends to make the electrical conductivity large. The dependence of electrical conductivity on S_T (Fig. 6(a)) is stronger than that on S_A (Fig. 6(b)) because the influence of N_T is greater than that of N_A , as shown in Eq. (5) and Eq. (7).

4.3 Temperature dependence of electrical conductivity

The temperature dependence of the electrical conductivity is shown in Fig. 8. S_T is taken as a parameter. The lines in Fig. 8 are the average values of calculated electrical conductivity for DC. The electrical conductivity increases with the increase of S_T over the entire range of temperature. The gradient of each line decreases as S_T increases. These results also indicate that the effective height of the Schottky barrier decreases, as seen in Eq. (7), with the increase of S_T . These results are also explained by the percolation theory,⁸⁾⁻¹⁰⁾ as noted in Section 4.2. The large S_T tends to make the variation of Φ_B wide and many Φ_B have low barrier height (low Φ_B). The current flows through the path, formed only by the low Φ_B , with a certain probability, and then tends to make the electrical conductivity large. These findings also mean that the sensitivity of the material when used as a thermistor decreases due to the nonuniformity of the microstructure.

Fig. 8. Temperature dependence of electrical conductivity.

5. Conclusions

In order to estimate the effects of the nonuniformity of the SiC ceramic semiconductor microstructure on the electrical conductivity, several simulations in which S_T and S_A were used as the parameters were performed. From the results of these simulations, the following were revealed.

(1) The electrical conductivity has a frequency dependence and it shows good agreement with the measured results.

(2) Increasing S_T or S_A tends to increase the electrical conductivity itself and the width of the variation of the electrical conductivity in the low-frequency region. These tendencies were explained by the percolation theory.

(3) Increasing S_T or S_A tends to decrease the sensitivity of the material when used as a thermistor.

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