Temperature dependences of current density–voltage and capacitance–frequency characteristics of hydrogenated nanocrystalline cubic SiC/crystalline Si heterojunction diodes.

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Abstract

We investigated the temperature dependences of the current density–voltage $(J-V)$ and capacitance–frequency $(C-f)$ characteristics of hydrogenated nanocrystalline cubic SiC/crystalline Si heterojunction diodes. The $J-V$ characteristics showed that over the measured temperature range (100–400 K) the carrier transport was governed by diffusion and recombination. Recombination became dominant with decreasing temperature and tunneling did not contribute to the carrier transport. The $C-f$ characteristics showed two relaxation processes dominant at low and high temperatures. The relaxation process dominant at low temperatures had different relaxation times depending on the heterojunction diode, which was caused by shallow states with different densities. The relaxation process dominant at high temperatures had almost the same relaxation times among diodes, which was caused by deep states (0.25–0.27 eV) with almost the same densities.

Keywords

Silicon carbide, nanocrystalline, hot-wire chemical vapor deposition, heterojunction, current density–voltage characteristics, capacitance–frequency characteristics

1. Introduction

Hydrogenated nanocrystalline cubic silicon carbide (nc-3C-SiC:H) is a wide-bandgap semiconductor composed of nanoscale SiC crystallites and an amorphous SiC:H phase [1], and has been expected to possess similar properties to crystalline SiC [2]. Therefore, nc-3C-SiC:H has gained much attention for its potential use as the emitter layer in solar cells [3,4]. Unlike crystalline SiC [5], nc-3C-SiC:H can be fabricated with low-temperature processes (<400 °C) such as chemical vapor deposition (CVD) [3,6] and magnetron sputtering [7], which reduces thermal damage to the substrates and decreases the cost of fabricating the solar cells. Among these fabrication techniques, hot-wire CVD (HW-CVD) is the most promising because it easily generates a high density of hydrogen radicals [8], which play an important role in nucleation and growth of nanocrystallites [9], and does not generate ions, which damage the substrate and the surface of the growing film [10]. We have fabricated nc-3C-SiC:H with HW-CVD by using a $SiH_4/CH_4/H_2$ mixture gas [1,11-16], and, successively, n-type nc-3C-SiC:H by using N_2 as a dopant gas [17], and we have studied the relationship between its fabrication conditions and material properties.

Recently, we deposited n-type nc-3C-SiC:H on p-type crystalline Si (c-Si) to fabricate nc-3C-SiC:H/c-Si heterojunction diodes and investigated how the H_2 gas flow rate affected the current density–voltage ($J-V$) and the admittance characteristics of the nc-3C-SiC:H/c-Si heterojunction diodes [18]. These characteristics indicated that interfacial defect density increased with increasing the H_2 gas flow rate. This resulted from damage to the c-Si surface by excess H radicals during the initial stage of the nc-3C-SiC:H layer deposition [18]. However, the effect of the interfacial defects on the transport mechanism is not clear. In the present study, we investigate the temperature dependences of the $J-V$ and admittance characteristics of nc-3C-SiC:H/c-Si heterojunction diodes, and discuss their transport mechanism and how interfacial defects affect them.

2. Experimental details

The heterojunction diodes were fabricated by depositing a layer of n-type nc-3C-SiC:H on c-Si wafer chips by using HW-CVD [18]. The wire was a W filament with a diameter of 0.4 mm and a length of 60 mm, folded into a 100-mm-long section. The distance between the wire and the substrates was 26 mm. SiH_4 and CH_4 source gases and an N_2 dopant gas were used with flow rates of 1, 1, and 50 sccm, respectively. These gases were diluted with H_2 at 200 and 1000 sccm. The total gas pressure was 530 Pa. The wire temperature was 1800 °C. Prior to depositing the nc-3C-SiC:H layer, the c-Si wafer chips were dipped in diluted hydrofluoric acid (2%, 60 s) to remove the native surface oxide. After the nc-3C-SiC:H layer was deposited, Al electrodes were deposited on both sides of the diode by using thermal evaporation, and then an H-radical treatment was performed [18].

The current–voltage characteristics were measured with a source-meter (Keithley, 2401). The admittance characteristics were measured with an LCR meter (NF Corporation, ZM2353). These measurements were performed in a cryogenic system under vacuum at temperatures of 100–400 K.

3. Results and Discussion

3.1 Current density–voltage characteristics

Figure 1 shows the current density–voltage ($J-V$) characteristics for the two types of nc-3C-SiC:H/c-Si heterojunction diodes measured at various temperatures T. These diodes were fabricated with H_2 gas flow rates of 200 and 1000 sccm, denoted as HJ-A and HJ-B, respectively. The crystallinity of nc-3C-SiC thin films was estimated by examining the Si–C stretching (Si–C(st)) infrared absorption peak (~800 cm^{-1}) [1,11–14]. As reported previously [18], the full width at half maximum of the Si–C(st) peak decreased from ~86 to ~76 cm^{-1} as the H_2 gas flow rate increased from 200 to 1000 sccm, while the intensity of the Si–C(st) peak remained almost constant ($\sim 6 \times 10^4$ cm^{-1}). Meanwhile, the ideality factor at room temperature increased from ~1.5 to ~1.8 with increasing H_2 gas flow rate [18]. These results mean that the crystallinity of the nc-3C-SiC:H layer in the HJ-A diode was lower than that in the HJ-B diode, while the diode characteristics of the HJ-A diode were better than those of the HJ-B diode [18].

The $J-V-T$ characteristics of these heterojunction diodes are similar to those of hydrogenated amorphous Si (a-Si:H)/c-Si heterojunction diodes [19]; a linear region appeared in the forward bias region in the semilogarithmic plot of each $J-V$ curve, and this region shifted to a lower bias voltage with increasing temperature. In general, the $J-V$ curves of pn junction diodes are described as

$$J = J_0 \left[\exp\left(\frac{q(V - JR_\mathrm{s})}{nkT} \right) - 1 \right] + \frac{V - JR_\mathrm{s}}{R_\mathrm{sh}} \qquad (1)$$

where n is the ideality factor, J_0 is the reverse saturation current density, R_s is the series resistance, R_sh is the shunt resistance, q is the elementary charge, and k is the Boltzmann constant. As we have done previously [18], we evaluated n and R_s from the vertical and horizontal intercepts, respectively, of the $G/J-G$ plot, where G is the small-signal conductance given by $G = dJ/dV$ [20,21]. The values of J_0 were evaluated by fitting $J-V$ curves at forward bias with the obtained values of n and R_s.

The values of R_s are on the order of 10^{-1} $\Omega\mathrm{cm}^2$ and independent of temperature for all the heterojunction diodes investigated in the present study. The temperature independence indicates that these values of R_s come from features other than the characteristics of the heterojunction diodes. Therefore, R_s will not be discussed further.

Figure 2(a) shows the ideality factor, n, as a function of the temperature. For the HJ-A diode, n increased monotonically from 1.23 to 1.94 as the temperature decreased from 400 to 100 K. This finding indicates that diffusion was the dominant transport mechanism at high temperature, and that recombination became dominant as the temperature decreased and was the main transport mechanism at low temperature [22–25]. Similarly, for the HJ-B diode, n increased with decreasing temperature.

However, n was 1.73 at 400 K, indicating that recombination was dominant even at high temperature. Moreover, n was >2 at temperatures below 200 K. This result suggests that tunneling may have been a significant transport mechanism. To confirm whether the tunneling contributed to transport, we estimated an exponential factor A given by the following formula:

$$J = J_0\left[\exp\left(A(V - JR_s)\right) - 1\right]. \qquad (2)$$

When transport is dominated by tunneling, A is independent of temperature [19,25]. Figure 2(b) shows A as a function of temperature. The A of the HJ-B diode depended on temperature, though its dependence was weaker than that of the HJ-A diode. This result indicates that tunneling did not contribute to transport in the HJ-B diode. This is true for the nc-3C-SiC:H/c-Si heterojunction diodes investigated in the present study.

The saturation current density, J_0, also offers insight into the transport mechanism. The J_0 of pn junction diodes is given by

$$J_0 = J_{00}\exp\left(-\frac{E_a}{nkT}\right) \qquad (3)$$

where J_{00} is the pre-exponential factor and E_a is the activation energy [21,26]. When the transport mechanism is a diffusion and/or recombination process, E_a is equal to the bandgap energy, E_g, of a narrow-bandgap semiconductor. Figure 3 shows the saturation current density raised to a power of the ideality factor, ${J_0}^n$, as a function of the reciprocal of kT. As shown in Fig. 3, the ${J_0}^n - 1/kT$ semilogarithmic plots show a linear relationship over the whole range of measured temperatures. This is true for all of the heterojunction diodes, including the HJ-A and the HJ-B diodes, investigated in the present study. The activation energies evaluated from the slopes of the straight lines are 1.11$\pm$0.06 eV, which is close to the bandgap of c-Si (E_g=1.12 eV). These findings indicate that diffusion and recombination is a predominant transport mechanism over the whole measured temperature range for all of the heterojunction diodes investigated in the present study. In other words, carrier transport via tunneling in these diodes is very unlikely, even in the HJ-B diode, which has a higher defect density than the HJ-A diode.

3.2 Capacitance–frequency characteristics

The following capacitance behaviors have been reported for a-Si:H/c-Si heterojunction diodes: (1) their capacitances are independent of frequency and increase gradually with increasing temperature, or (2) the capacitances rapidly increase (capacitance step) at moderate temperatures and the capacitance step shifts to higher temperatures as frequency increases, although the capacitances are independent of frequency at lower and higher temperatures [27,28]. The capacitance behaviors of the present nc-3C-SiC:H/c-Si heterojunction diodes, however, are different from those of the a-Si:H/c-Si heterojunction diodes. Figures 4 and 5 show the (a) frequency dependence and (b) the temperature dependence of the capacitance of the HJ-A and the HJ-B diodes, respectively. As shown in Figs. 4(a) and 5(a), at all measured temperatures the capacitances decreased monotonically with increasing frequency. At low frequencies ($f \leq 10$ kHz), the capacitances were almost independent of frequency, except for the HJ-A diode at low temperatures. Such frequency-independent capacitance values include the capacitance due to interfacial states [29]. At high frequencies ($f \geq 1$ MHz), the capacitances approached the values of the depletion layer capacitance, C_{D}. As shown in Fig. 4(b), at low frequencies ($f \leq 1$ kHz) the capacitances of the HJ-A diode increased with increasing temperature from 100 to 150 K and decreased with increasing temperature from 250 to 370 K. The HJ-B diode showed a similar temperature dependence of capacitance at low frequencies ($f \leq 10$ kHz, Fig. 5 (b)), although the dependence was much weaker than that of the HJ-A diode. At high frequencies ($f \geq 1$ MHz), the capacitances of the HJ-A diode increased gradually with increasing temperature and exhibited no step-like increases (Fig. 4(b)). Meanwhile, for the HJ-B diode, the capacitances over the same frequency range rapidly increased at temperatures above 300 K (Fig. 5(b)). These behaviors of the temperature-dependent capacitances were also caused by interfacial states.

The capacitance behaviors of the nc-3C-SiC:H/c-Si heterojunction diodes can be explained by the equivalent circuit shown in Fig. 6, where C_{D} is the depletion layer capacitance, and C_{is} and R_{is} are the capacitance and resistance, respectively, associated with interfacial states [29]. Taking it into account that interfacial states have an energy distribution, the measured capacitance, C_{m}, follows the Cole–Cole equation [30,31]:

$$C_{\mathrm{m}} = C_{\mathrm{D}} + \frac{C_{\mathrm{is}}}{2} \cdot \left\{ 1 - \frac{\sinh(\beta x)}{\cosh(\beta x) + \cos(\beta \pi / 2)} \right\} \tag{4}$$

$$x = \ln(\omega \tau_0) \tag{5}$$

$$\tau_0 = C_{\mathrm{is}} R_{\mathrm{is}} \tag{6}$$

where ω is the angular frequency, β is a parameter that indicates the degree of the relaxation-time distribution, and τ_0 is the average relaxation time. By fitting the $C_{\mathrm{m}} - f$ curves with Eq. (4), we evaluated C_{D}, C_{is}, τ_0, and β. Figure 7 shows (a) τ_0 versus the reciprocal of kT and (b) the relationship between τ_0 and C_{is}. τ_0 and C_{is} both decreased with increasing temperature. As shown in Figure 7(b), C_{is} was proportional to the square root of τ_0 ($C_{\mathrm{is}} \propto {\tau_0}^{1/2}$), giving rise to $R_{\mathrm{is}} = \tau_0/C_{\mathrm{is}} \propto {\tau_0}^{1/2}$. The decrease in C_{is} was caused by the decrease in the number of trapped carriers with increasing temperature.

The decreases in τ_0 and C_{is} with increasing temperature caused the capacitance behavior of the HJ-A diode at low frequencies ($f = 500\mathrm{Hz} - 1\mathrm{kHz}$); the capacitance first increases with increasing temperature and then decreases with further increasing temperature. At lower temperatures, C_{m} is smaller than $C_{\mathrm{is}} + C_{\mathrm{D}}$ because of the longer τ_0. Therefore, C_{m} increases with increasing temperature from 100 K to 150 K. This behavior means that the number of the trapped carriers responding to the low-frequency AC signal increases. At higher temperatures, C_{m} is almost equal to $C_{\mathrm{is}} + C_{\mathrm{D}}$ because of the shorter τ_0. Therefore, C_{m} decreases with increasing temperature. This is caused by the decrease in C_{is}, itself caused by the decrease in the number of trapped carriers. The C_{m} of the HJ-B diode at low frequencies ($f = 500\mathrm{Hz} - 10\mathrm{kHz}$) shows a weaker temperature dependence, which occurs because the HJ-B diode has a higher density of shallow interfacial states than the HJ-A diode. This will be discussed next.

Figure 7(a) shows that two relaxation processes exist. The relaxation times that are dominant at low and high temperatures are denoted by τ_{l} and τ_{h}, respectively. These are given by

$$1/\tau_0 = 1/\tau_{\mathrm{l}} + 1/\tau_{\mathrm{h}} \qquad (7)$$

$$\tau_{\mathrm{i}} = \tau_{\mathrm{i0}} \exp\left(E_{\mathrm{a\_i}}/kT\right) \qquad (8)$$

where τ_{i0} and $E_{\mathrm{a\_i}}$ (i = l or h) are the pre-exponential factor and the activation energy, respectively. By fitting $\tau_0 - 1/kT$ curves with Eqs. (7) and (8), we evaluated the values of the pre-exponential factors and the activation energies. For the HJ-A diode, $E_{\mathrm{a\_l}} = 23\ \mathrm{meV}$, $\tau_{\mathrm{l0}} = 3.8 \times 10^{-5}\ \mathrm{s}$, $E_{\mathrm{a\_h}} = 0.28$ eV, and $\tau_{\mathrm{h0}} = 2.9 \times 10^{-1}$ s; for the HJ-B diode, $E_{\mathrm{a\_l}} \simeq 3$ meV, $\tau_{\mathrm{l0}} = 3.4 \times 10^{-6}$ s, $E_{\mathrm{a\_h}} = 0.25$ eV, and $\tau_{\mathrm{h0}} = 2.0 \times 10^{-9}$ s. As shown in Fig. 7(a), the τ_{l} of the HJ-B diode was lower than that of the HJ-A diode by one to two orders of magnitude, while the τ_{h} values are on the same order. These findings suggest that the HJ-B diode has a higher density of shallow interfacial states than the HJ-A diode, while they have almost the same densities of deep interfacial states.

The apparent built-in voltages, $V_{\mathrm{D}}^{\mathrm{app}}$, were estimated from the horizontal intercept of the linear relationship of the $1/C_D^2 - V$ plots [18,32,33]. Figure 8 shows $V_{\mathrm{D}}^{\mathrm{app}}$ as a function of temperature. For the HJ-B diode, the $1/C_D^2 - V$ plots do not show a linear relationship at temperatures above 345 K, so $V_{\mathrm{D}}^{\mathrm{app}}$ cannot be estimated. The $V_{\mathrm{D}}^{\mathrm{app}}$ of the HJ-A diode decreases with increasing temperature. At low temperatures, most of the interfacial states trap carriers. Therefore, the interface states are almost neutral. As the temperature increases, the trapped carriers are released from the interfacial states, and the number of charged states, which do not trap carriers, increases. This causes the decrease in $V_{\mathrm{D}}^{\mathrm{app}}$, which follows this formula:

$$V_{\mathrm{D}}^{\mathrm{app}} = V_{\mathrm{D}} - BQ_{\mathrm{IS}}{}^{2} \tag{9}$$

where V_{D} is the built-in voltage, Q_{IS} is the charge of the interfacial states per unit area, and B is a constant [18,29]. The $V_{\mathrm{D}}^{\mathrm{app}}$ of the HJ-B diode also decreases with increasing temperature. However, the decrement is small, and all $V_{\mathrm{D}}^{\mathrm{app}}$ values of the HJ-B diode are close to that at high temperature of the HJ-A diode. This behavior results from the larger density of shallow interfacial states in the HJ-B diodes, as mentioned before. Most of these states do not trap carriers over the whole temperature range because of the shallow states, and they are charged. Therefore, $|Q_{\mathrm{IS}}|$ is large and $V_{\mathrm{D}}^{\mathrm{app}}$ is low.

4. Conclusion

We studied the temperature dependences of the $J-V$ and the $C-f$ characteristics of nc-3C-SiC:H/c-Si heterojunction diodes. The $J-V$ characteristics revealed that diffusion and recombination was the dominant carrier transport mechanism at 100–400 K for all of the nc-3C-SiC:H/c-Si heterojunction diodes fabricated with various H_2 gas flow rates and that tunneling did not contribute to the carrier transport. However, increasing the H_2 gas flow rate increased the interfacial defect density, which caused recombination to be the dominant carrier transport mechanism. The $C-f$ characteristics showed that two relaxation processes were involved: deep and shallow interfacial states. The density of deep interfacial states was almost the same among all of the nc-3C-SiC:H/c-Si heterojunction diodes. However, the density of shallow interfacial states increased with increasing H_2 gas flow rate, shortening the relaxation time.

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Figure captions

Figure 1 Current density–voltage characteristics for (a) HJ-A and (b) HJ-B measured at 100, 150, 200, 250, 270, 286, 303, 323, 345, 370, and 400 K.

Figure 2 (a) Ideality factor, *n*, and (b) exponential factor, *A*, as functions of temperature. The lines are visual guides.

Figure 3 Saturation current density raised to a power of the ideality factor, *n*, as a function of 1/kT for (a) HJ-A and (b) HJ-B.

Figure 4 (a) Frequency dependence and (b) temperature dependence of the capacitance of the HJ-A diode. The lines are visual guides.

Figure 5 (a) Frequency dependence and (b) temperature dependence of the capacitance of the HJ-B diode. The lines are visual guides.

Figure 6 Equivalent circuit of the heterojunction diode. C_{D} is the depletion-layer capacitance. C_{is} and R_{is} are the capacitance and the resistance, respectively, associated with interfacial states [29].

Figure 7 (a) τ_0 versus the reciprocal of kT and (b) the relationship between τ_0 and C_{is}. The lines in (a) are calculated based on Eqs. (7) and (8). The lines in (a) were calculated using Eqs. (7) and (8) with $E_{\mathrm{a\_l}} = 23$ meV, $\tau_{\mathrm{l0}} = 3.8 \times 10^{-5}$ s, $E_{\mathrm{a\_h}} = 0.28$ eV, and $\tau_{\mathrm{h0}} = 2.9 \times 10^{-10}$ s for the HJ-A diode (red lines) and $E_{\mathrm{a\_l}} \simeq 3$ meV, $\tau_{\mathrm{l0}} = 3.4 \times 10^{-6}$ s, $E_{\mathrm{a\_h}} = 0.25$ eV, and $\tau_{\mathrm{h0}} = 2.0 \times 10^{-9}$ s for the HJ-B diode (blue lines). The lines in (b) show the relationship $C_{\mathrm{is}} \propto {\tau_0}^{1/2}$.

Figure 8 Apparent built-in voltages as a function of temperature. The lines are visual guides.