Transition of conduction mechanism from band to variable-range hopping conduction due to Al doping in heavily Al-doped 4H-SiC epilayers

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To realize excellent SiC n-channel insulated-gate bipolar transistors (IGBTs), it is crucial to fabricate thick p-type SiC substrates (i.e. the collectors of IGBTs) with very low resistance and good crystalline quality because the on-resistance of SiC IGBTs is considerably lower than that of commercially available SiC n-channel metal–oxide–semiconductor field-effect transistors. To reduce the resistance of these materials, elucidation of the underlying conduction mechanisms is essential. The electrical transport properties of heavily Al-implanted 4H-SiC layers, Al-doped 6H-SiC wafers, and Al-doped 4H-SiC epilayers have been reported. We have also investigated the temperature dependence of resistivity [\(\rho(T)\)] for heavily Al-doped 4H-SiC epilayers. We reported that in epilayers with Al concentrations \(C_{\text{Al}}\) of \(\leq 1.5 \times 10^{20}\) cm\(^{-3}\) the dominant conduction mechanisms at high and low temperatures were band and nearest-neighbor hopping (NNH) conduction, respectively, and in epilayers with \(C_{\text{Al}}\) values of \(\geq 2.4 \times 10^{20}\) cm\(^{-3}\) the dominant conduction mechanism was variable-range hopping (VRH) conduction over the entire range of measurement temperatures examined. In this study, we investigated the transition of the conduction mechanism from band and NNH conduction to VRH conduction at \(C_{\text{Al}}\) values of approximately \(2 \times 10^{20}\) cm\(^{-3}\). Al-doped 4H-SiC epilayers with a thickness of approximately 90 \(\mu\)m were grown using a horizontal hot-wall CVD system (VP508 GFR, Aixtron) at about 1620 °C on (0001)-oriented 3 inch n-type 4H-SiC wafers (8° off-oriented toward [1120]). Four Al/Ti/Al contact dots in the van der Pauw configuration were deposited by electron beam evaporation of Al and Ti, and the samples were then annealed at 1000 °C under N\(_2\) atmosphere. Four beam epilayers were obtained with \(C_{\text{Al}}\) values of \(9.6 \times 10^{19}\), \(1.5 \times 10^{20}\), \(1.8 \times 10^{20}\), and \(3.5 \times 10^{20}\) cm\(^{-3}\), as determined by secondary-ion mass spectrometry. The FWHM values of the X-ray rocking curves (XRCs) were measured using a high-resolution X-ray diffraction (Panalytical X’Pert MRD) system. Their \(\rho(T)\) values in the range of 20–600 K were measured via the van der Pauw method using a ResiTest8400 system (TOYO Corporation). The technique used to obtain reliable \(\rho(T)\) values was reported in our previous paper.

The well-known conduction mechanisms in semiconductors include band conduction, NNH conduction, and VRH conduction. Figures 1(a) and 1(b), respectively, show the density-of-states distribution and energy band diagram for an Al-doped 4H-SiC epilayer. With increasing \(C_{\text{Al}}\), the distance between nearest-neighbor Al sites decreases and density of localized states increases.

Fig. 1. (Color online) (a) Density-of-states distribution and (b) energy band diagram for an Al-doped 4H-SiC epilayer. With increasing \(C_{\text{Al}}\), the distance between nearest-neighbor Al sites decreases and density of localized states increases.

We investigate the transition of the conduction mechanism from band and nearest-neighbor hopping (NNH) conduction to variable-range hopping (VRH) conduction in heavily Al-doped 4H-SiC epilayers with increasing Al concentration \((C_{\text{Al}})\). In a sample with \(C_{\text{Al}}\) of \(1.8 \times 10^{20}\) cm\(^{-3}\), the dominant conduction mechanisms at high and low temperatures were band and VRH conduction, respectively, whereas in samples with lower \(C_{\text{Al}}\) values they were band and NNH conduction, respectively, and in samples with higher \(C_{\text{Al}}\) values VRH conduction was dominant over the entire range of measurement temperatures examined (20–600 K). © 2019 The Japan Society of Applied Physics

Fig. 1. (Color online) (a) Density-of-states distribution and (b) energy band diagram for an Al-doped 4H-SiC epilayer. With increasing \(C_{\text{Al}}\), the distance between nearest-neighbor Al sites decreases and density of localized states increases.

The well-known conduction mechanisms in semiconductors include band conduction, NNH conduction, and VRH conduction. Figures 1(a) and 1(b), respectively, show the density-of-states distribution and energy band diagram near the top of the valence band (VB) \((E_V)\) for an Al-doped 4H-SiC epilayer. In the case of low \(C_{\text{Al}}\), only the holes in the VB can flow, which corresponds to band conduction, because the distance between nearest-neighbor Al acceptor sites is too great for the holes at Al acceptor sites to hop. In contrast, in the case of high \(C_{\text{Al}}\), the holes at Al acceptor sites can hop to their unoccupied nearest-neighbor Al sites owing to the smaller distance between Al acceptor sites, leading to NNH conduction. At very high levels of Al doping, local lattice distortion is considered to increase as a result of doping-induced strain, which may lead to local disturbance of the periodicity of the lattice. This indicates that localized states must be created in the bandgap near the delocalized states, that is, the VB and conduction band (CB). Because the Fermi level \((E_F)\) was reported to be located between \(E_V\) and an Al acceptor level \((E_{\text{Al}})\) even at high temperatures in the case of heavily Al-doped 4H-SiC, the

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there must exist localized states around $E_F$, as depicted in Fig. 1(a). Figure 1(b) shows that holes at localized states around $E_F$ can hop to unoccupied localized states around $E_F$, which corresponds to VRH conduction. As the currents due to band, NNH, and VRH conduction flow completely in parallel in the VB, $E_{AI}$ and $E_F$, respectively, $\rho(T)$ can be expressed as\(^{(12)}\)

$$\frac{1}{\rho(T)} = \frac{1}{\rho_{\text{band}}(T)} + \frac{1}{\rho_{\text{NNH}}(T)} + \frac{1}{\rho_{\text{VRH}}(T)},$$

(1)

$$\rho_{\text{band}}(T) = \rho_{\text{band}0} \exp\left(\frac{\Delta E_{\text{band}}}{k_B T}\right),$$

(2)

$$\rho_{\text{NNH}}(T) = \rho_{\text{NNH}0} \exp\left(\frac{\Delta E_{\text{NNH}}}{k_B T}\right),$$

(3)

and

$$\rho_{\text{VRH}}(T) = \rho_{\text{VRH}0} \exp\left[\left(\frac{T_0}{T}\right)^{1/4}\right],$$

(4)

where $\rho_{\text{band}}(T)$, $\rho_{\text{NNH}}(T)$, and $\rho_{\text{VRH}}(T)$ are the $\rho(T)$ for band, NNH, and VRH conduction, respectively; $\rho_{\text{band}0}$, $\rho_{\text{NNH}0}$, and $\rho_{\text{VRH}0}$ are the pre-exponential factors for band, NNH, and VRH conduction, respectively; $\Delta E_{\text{band}}$ and $\Delta E_{\text{NNH}}$ are the activation energies for band and NNH conduction, respectively; $T_0$ is a constant for VRH conduction; and $k_B$ is the Boltzmann constant. It is readily apparent from Eq. (1) that at a given $T$ the conduction mechanism with the lowest resistivity becomes dominant.

Figure 2 shows Arrhenius plots of $\rho(T)$ for the epilayers with $C_{AI}$ values of $9.6 \times 10^{19}$ ($\diamond$), $1.5 \times 10^{20}$ ($\Box$), and $1.8 \times 10^{20}$ cm$^{-3}$ ($\bigtriangleup$). According to Eqs. (2) and (3), the solid straight lines for the three samples correspond to band conduction, whereas the broken straight lines for the samples with $C_{AI}$ values of $9.6 \times 10^{19}$ and $1.5 \times 10^{20}$ cm$^{-3}$ indicate NNH conduction. In contrast, for the sample with $C_{AI}$ of $1.8 \times 10^{20}$ cm$^{-3}$, as indicated by the dotted line, it is apparent that the data at low temperatures cannot be adequately approximated by a straight line, indicating that the conduction mechanism at low temperatures is another type of hopping conduction rather than NNH conduction, whereas the data at high temperatures can be, indicating that the conduction mechanism at high temperatures is band conduction.

Figure 3 shows $\rho(T) = T^{-1/4}$ plots for the 4H-SiC epilayers with $C_{AI}$ values of $1.8 \times 10^{20}$ ($\bigtriangleup$) and $3.5 \times 10^{20}$ cm$^{-3}$ ($\bigtriangleup$). According to Eq. (4), the solid straight lines correspond to VRH conduction. For the sample with $C_{AI}$ of $3.5 \times 10^{20}$ cm$^{-3}$, the conduction mechanism was found to be VRH conduction over the entire range of measurement temperatures. In contrast, for the sample with $C_{AI}$ of $1.8 \times 10^{20}$ cm$^{-3}$, the conduction mechanism was only VRH conduction at low temperatures, whereas the data could be adequately approximated by a straight line. Consequently, the dominant conduction mechanisms in the sample with $C_{AI}$ of $1.8 \times 10^{20}$ cm$^{-3}$ at high and low temperatures were found to be band and VRH conduction, respectively. Therefore, upon increasing $C_{AI}$, the conduction mechanism at low temperatures changes from NNH to VRH conduction, and then finally the conduction mechanism becomes VRH conduction over the entire range of measurement temperatures.
was reported to be located between axis increased with increasing c axis, whereas the lattice constant a remained almost unchanged. These observations can be ascribed to the larger covalent radius of a substitutional Al atom (0.125 nm) compared with a Si atom (0.117 nm). As a result, high levels of Al doping are considered to induce local disturbance of the periodicity of the 4H-SiC lattice, implying an increase in the density of localized states near VB and CB in the bandgap. Because EF was reported to be located between EV and EAl in heavily Al-doped 4H-SiC even at high temperatures, there must exist localized states around EF. Therefore, as CAI increases, \( \rho_{VRH}(T) \) becomes lower than \( \rho_{NNH}(T) \) and VRH conduction becomes dominant at low temperatures according to Eq. (1). Al doping was reported to reduce the hole mobility in the VB for Al-doped 4H-SiC, because neutral impurity scattering becomes dominant instead of acoustic phonon scattering in heavily Al-doped 4H-SiC, where neutral impurities are neutral Al acceptors, suggesting that the decrease in \( \rho_{\text{band}}(T) \) is reduced although the hole concentration in Al-doped 4H-SiC is increased with increasing CAI. Consequently, \( \rho_{VRH}(T) \) becomes lower than \( \rho_{\text{band}}(T) \) at high temperatures. Finally, VRH conduction becomes dominant over the entire range of measurement temperatures.

In summary, high levels of Al doping decrease \( \rho_{VRH}(T) \). In samples with \( CAI \) values of approximately \( 1 \times 10^{20} \text{cm}^{-3} \), the dominant conduction mechanisms at high and low temperatures are band and NNH conduction, respectively. With increasing \( CAI \), however, VRH conduction first becomes the dominant conduction mechanism rather than NNH conduction at low temperatures, and then finally becomes the dominant conduction mechanism over the entire range of measurement temperatures (20–600 K).

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