ESR study of localized and delocalized electrons in nitrogen-doped 6H SiC crystals

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We have studied the temperature behavior of the electron spin resonance (ESR) spectra of nitrogen (N) donors in n-type 6H polytype of silicon carbide (SiC) crystals grown by Lely and sublimation sandwich methods (SSM) with a donor concentration of about $(N_D - N_A) \approx 10^{17}$ cm^{-3} at $T = 60$-150 K. The broad ESR signal with Lorentzian lineshape and $g_{\|} = 2.0043(3)$, $g_{\perp} = 2.0030(3)$ appeared in the ESR spectrum at $T > 80$ K was reassigned. This line was observed previously in [1, 2] and was attributed to N in the thermally excited antisymmetric 1s(E) state. Based on the analysis of the ESR lineshape, linewidth and *g*-tensor of the observed single broad line, we have attributed it to the conduction electrons (CE) appeared in the ESR spectrum of the n-type 6H SiC at high temperatures due to the ionization of the electrons from ground 1s(A_1) and excited 1s(E) state of the N donors to the conduction band.

We have found that the temperature dependence of CE ESR linewidth is described by the exponential law (Orbach process) in the temperature range from 80 K to 150 K with the activation energy corresponding to the energy separation between 1s(A_1) and 1s(E) energy levels for N donors at quasi-cubic "k1" and "k2" sites ($N_{k1,k2}$). The exponential increase of the CE ESR linewidth with the temperature is explained by coupling of the CE with the spin system of localized electrons.

The observed reduction of the hyperfine (hf) splitting for the $N_{k1,k2}$ donors at $T > 75$ K with the temperature increase has been explained by electron jumping over the donor states, resulting in the fluctuation of local field (averaging of the hf interaction) determined by the temperature-dependent correlation time of fluctuations.

The electrical characteristics of both n-type 6H SiC samples were studied by the contact-free MW conductivity method. From the theoretical analysis of the temperature variation of the ESR cavity *Q*-factor loaded with n-type 6H SiC samples we have found that the ionization of free electrons in the conduction band occurs from the $N_{k1,k2}$ energy levels in Lely grown sample and from N_h energy level in 6H SiC sample grown by SSM. The ionization of free electrons from the different energy levels in two samples can be explained by the different position of the Fermi level and amounts of the distant donor pairs formed between N atoms residing at quasi-cubic and hexagonal sites in two samples. A small amount of the distant pairs in 6H SiC grown by SSM gives rise to the significantly higher concentration of the shallow N donors substituting hexagonal ("h") position (N_h) in the isolated electrically active state and as a result leads to the ionization of the free electrons from N_h energy level to the conduction band.

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