A graphical peak analysis method for characterizing impurities in diamond from temperature-dependent majority-carrier concentration

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Using a temperature-dependent majority-carrier concentration (i.e., n(T) for electrons or p(T) for holes), the density and energy level of impurities are usually evaluated from $\ln n(T) - 1/T$ or $\ln p(T) - 1/T$ curve. However, this analysis cannot be applied in semiconductors with more than two types of impurity species or compensated semiconductors. Moreover, it is difficult to obtain reliable values by fitting a simulation to the experimental data, because it is necessary to assume the number of impurity species before the curve-fitting procedure.

Without any assumptions regarding impurity species, free carrier concentration spectroscopy (FCCS) can accurately determine the densities and energy levels of impurities. ^{1,2)} The FCCS signal is defined as^{1,2)}

$$H(T, E_{\rm ref}) \equiv \frac{n(T)^2}{(kT)^{5/2}} \exp\left(\frac{E_{\rm ref}}{kT}\right) \text{ or } H(T, E_{\rm ref}) \equiv \frac{p(T)^2}{(kT)^{5/2}} \exp\left(\frac{E_{\rm ref}}{kT}\right),$$

and has a peak at the temperature corresponding to each impurity level, where $E_{\rm ref}$ is the parameter that can shift the peak temperature of $H(T, E_{\rm ref})$ within the measurement temperature range. From each peak of $H(T, E_{\rm ref})$, the density and energy level of the corresponding impurity can be accurately determined.

Since the energy levels of substitutional acceptors in p-type SiC and GaN are deep, the distribution function $f_{\rm MC}(E_{\rm A})$ including the influence of the excited states of the acceptor is required to analyze their experimental p(T),^{2,3)} instead of the Fermi-Dirac distribution function $f_{\rm FD}(E_{\rm A})$ that does not include this influence.

In this paper, we report on our investigation of accurate evaluation of impurities in diamond by FCCS using several distribution functions for acceptors. A 1.73 -µm-thick p-type single crystalline diamond epilayer was grown on a synthesized single crystal 1b diamond, and the B-doping level ($C_{\rm B}$) was 2×10^{17} cm^{-3.4}. The p(T) was obtained by Hall-effect measurements in the van der Pauw configuration. Figure 1 shows p(T) and $H(T, E_{\rm ref})$ with $E_{\rm ref}$ of 0.31 eV, denoted by circles and triangles, respectively. Using $f_{\rm FD}(E_{\rm A})$, the acceptor density ($N_{\rm A}$) and energy level ($E_{\rm A}$), and the compensating density ($N_{\rm comp}$) were determined from the peak of $H(T, E_{\rm ref})$ as 9.7×10^{17} cm⁻³, $E_{\rm V} + 0.34$ eV, and 4.0×10^{16} cm⁻³, respectively. However, the determined $N_{\rm A}$ is approximately 5 higher than the $C_{\rm B}$. Using $f_{\rm MC}(E_{\rm A})$, on the other hand, those were determined as 2.8×10^{17} cm⁻³, $E_{\rm V} + 0.32$ eV, and 2.0×10^{16} cm⁻³, respectively. In this case, the determined $N_{\rm A}$ was close to the

this case, the determined N_A was close to the C_B , indicating that the effect of the excited states of the B acceptor in diamond on p(T) should not be ignored.

References

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Fig. 1. Temperature-dependent hole concentration and FCCS signal.