A GRAPHICAL PEAK ANALYSIS METHOD FOR CHARACTERIING IMPURITIES IN DIAMOND FROM TEMPERATURE-DEPEMDEMT MAJORITY-CARRIER CONCENTRATION

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Abstract.

From a temperature dependence of the majority-carrier concentration in a B-doped or P-doped diamond epilayer, the density and energy level of dopant are determined by a graphical peak analysis method (free carrier concentration spectroscopy: FCCS). Moreover, the influence of the excited states of the dopant on the majority-carrier concentration is investigated. The excited states of the B acceptor affect the hole concentration, indicating that the acceptor density determined using the experimentally obtained hole concentration strongly depends on whether the excited states of the acceptor are considered or not in the analysis. On the other hand, the excited states of the P donor do not affect the electron concentration very much.

Introduction

Analysis methods

ln n(T)-1/T or ln p(T)-1/T

The analysis of ln n(T)-1/T or ln p(T)-1/T curve cannot be applied to semiconductors with more than one types of impurities or compensated semiconductors.

Curve-fitting

It is difficult to obtain reliable densities and energy levels of impurities by fitting an n(T) or p(T) simulation to the experimental data, because it is necessary to assume the number of impurity species before the curve-fitting procedure.

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A graphical peak analysis method can determine the densities and energy levels of impurities without any assumptions regarding impurity species.

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Free Carrier Concentration Spectroscopy (FCCS)

Definition of FCCS [1,2]

$$H(T,E_{\mathrm{ref}}) \equiv \frac{n(T)^2}{k^{5/2}T^{5/2}} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right)$$

$$H(T,E_{\mathrm{ref}}) \equiv \frac{p(T)^2}{k^{5/2}T^{5/2}} \exp\left(\frac{E_{\mathrm{ref}}}{kT}\right)$$

The FCCS signal has a peak at the temperature corresponding to each impurity level.

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From each peak, the density and energy level of the corresponding impurity can be accurately determined.

Effect of excited states of dopant [3,4]

Fermi-Dirac distribution function

$$f_{\mathrm{FD}}(E_{\mathrm{A}}) = \frac{1}{1+4\exp\left(-\frac{E_{\mathrm{F}}(T)-E_{\mathrm{A}}}{kT}\right)}$$

Distribution function including the influence of the excited states of the acceptor

$$f(E_{\mathrm{A}}) = \frac{1}{1+g_{\mathrm{A}}(T)\exp\left(-\frac{E_{\mathrm{F}}(T)-E_{\mathrm{A}}}{kT}\right)}$$

Effective acceptor degeneracy factor

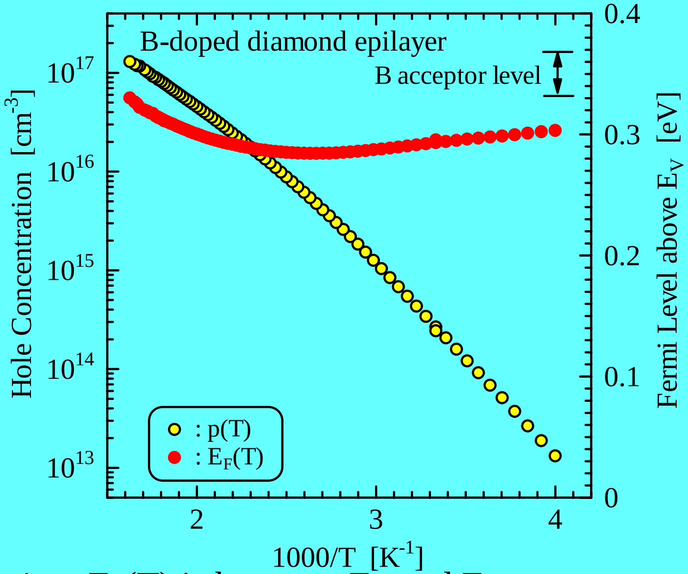
$$g_{\mathrm{A}}(T) = 4\left[1+\sum_{r=2} g_r \exp\left(\frac{E_r-E_{\mathrm{A}}}{kT}\right)\right]\exp\left(-\frac{\overline{E_{\mathrm{ex,A}}(T)}}{\mathrm{k}T}\right)$$

Ensemble average energy of holes at the ground and excited state levels

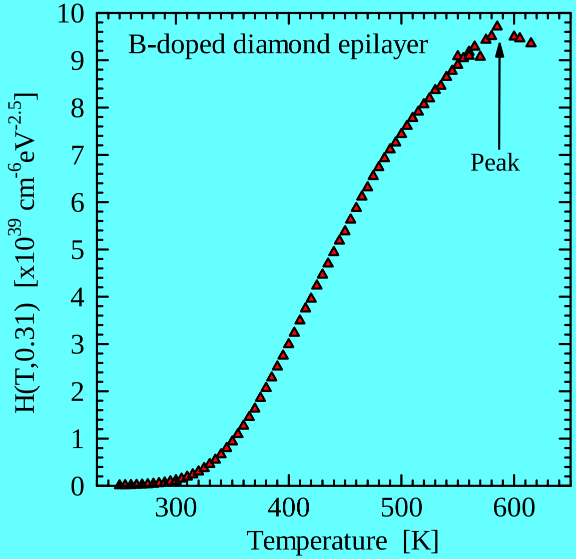
$$\overline{E_{\mathrm{ex,A}}(T)} = \frac{\sum_{r=2}(E_{\mathrm{A}}-E_r)g_r\exp\left(\frac{E_r-E_{\mathrm{A}}}{kT}\right)}{1+\sum_{r=2} g_r \exp\left(\frac{E_r-E_{\mathrm{A}}}{kT}\right)}$$

Results and Discussion

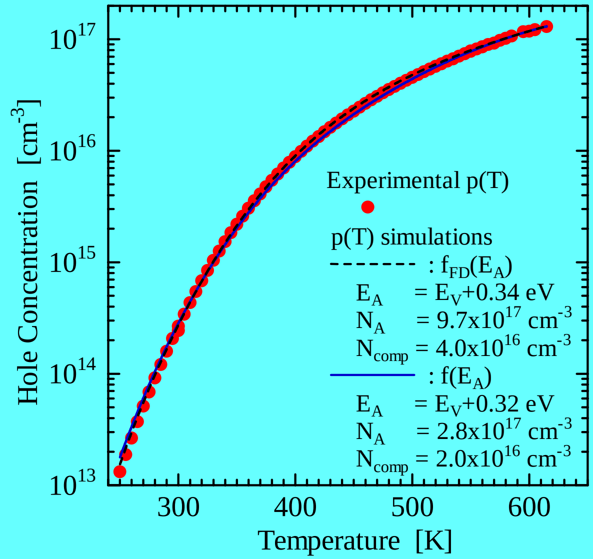
B-doped diamond



FCCS signal



p(T) simulations



1. E_F(T) is between E_A and E_V.
2. The difference between E_F(T) and excited states is close (~0.2 eV)

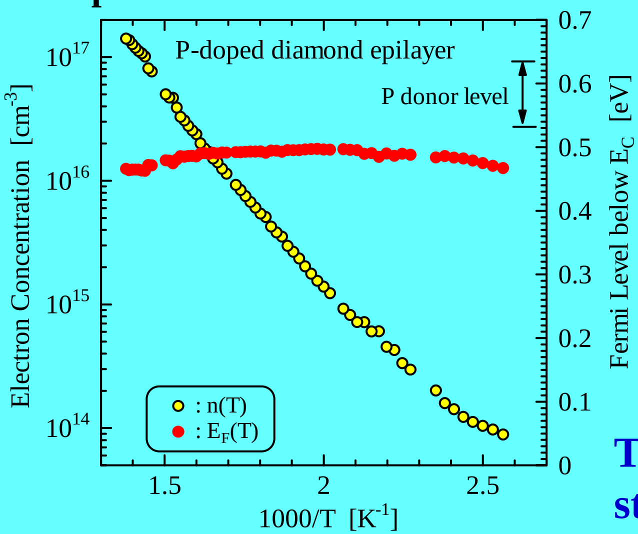
From the peak of FCCS signal, N_A is $9.7x10^{17}$ cm^{-3} for $f_{FD}(E_A)$, N_A is $2.8x10^{17}$ cm^{-3} for $f(E_A)$.

Although N_A for $f_{FD}(E_A)$ is ~3 times higher than N_A for $f(E_A)$, p(T) simulations are similar each other, and are in agreement with the experimental p(T).

The B concentration determined by SIMS was ~$2x10^{17}$ cm^{-3}.

The excited states of the B acceptor should affect p(T).

P-doped diamond



Although E_F(T) is between E_A and E_V, the difference between E_F(T) and excited states is much larger (~0.4 eV)

From the peak of FCCS signal, N_A is $2x10^{19}$ cm^{-3} for both $f_{FD}(E_A)$ and $f(E_A)$.

The effect of the excited states of the P donor is small.

Conclusion

In the analysis, the effect of the excited states of the B acceptor should have been considered. Even in the case that the excited states strongly affect the majority-carrier concentration, the density and energy level of the dopant could be determined by FCCS.

References

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