HPHT annealing of Ni-containing nitrogen-rich synthetic diamonds and the formation of NE8 centre

Liangchao Chen, Weixia Shen, Chao Fang*, Yuewen Zhang, Peiyang Mu, Guangtong Zhou, Qianqian Wang, Zhuangfei Zhang*, Xiaopeng Jia

Key Laboratory of Material Physics of Ministry of Education, School of Physics and Microelectronics, Zhengzhou University

Corresponding Author:*Email: fangchao1989@zzu.edu.cn; zhangzf@zzu.edu.cn.

The nitrogen concentrations in Table 2 are determined using the formula as follows:

The concentration of nitrogen only in the C-centre form (N_C) in diamond can be calculated from the absorption coefficient α_C/cm^{-1} of the peak at 1130 cm^{-1}[1] to be

$$N_C/10^{-6} = 25\ \alpha_C \tag{1}$$

The concentration of aggregated nitrogen only in the A-centre form (N_A) is determined by measuring the absorption coefficient α_A/cm^{-1} of the peak at 1282 cm^{-1}[2] to be

$$N_A/10^{-6} = 16.5\ \alpha_A \tag{2}$$

On the assumption that spectra are linearly overlapped, the concentration of A-centres and C-centres in mixed type of diamond IaA+Ib is still determined by the absorption coefficients α_C and α_A which are expressed in the terms of α_{1130} and α_{1282} [3] to be

$$\alpha_C = 1.1\ \alpha_{1130} - 0.2\ \alpha_{1282} \tag{3}$$

$$\alpha_A = 1.1\ \alpha_{1282} - 0.2\ \alpha_{1130} \tag{4}$$

where α_{1130} and α_{1282} are absorption coefficients of the peaks at 1130 cm^{-1} and 1282 cm^{-1}, respectively. The absorption coefficient of the peak at 2000 cm^{-1} is well known to be 12.3 cm^{-1}, so α_{1130} and α_{1282} can be obtained by comparing their absorption intensity (μ) with that of the peak at 2000 cm^{-1} as follows:

$$\alpha_{1130} = \mu(1130\ \mathrm{cm}^{-1})/\mu(2000\ \mathrm{cm}^{-1}) \times 12.3 \quad (5)$$

$$\alpha_{1282} = \mu(1282\ \mathrm{cm}^{-1})/\mu(2000\ \mathrm{cm}^{-1}) \times 12.3 \quad (6)$$

The values of absorption intensity are calculated according to the recorded value A in IR spectra to be

$$\mu(1130\ \mathrm{cm}^{-1}) = A(1130\ \mathrm{cm}^{-1}) - A(1370\ \mathrm{cm}^{-1}) \quad (7)$$

$$\mu(2000\ \mathrm{cm}^{-1}) = A(2000\ \mathrm{cm}^{-1}) - A(1370\ \mathrm{cm}^{-1}) \quad (8)$$

$$\mu(1282\ \mathrm{cm}^{-1}) = A(1282\ \mathrm{cm}^{-1}) - A(1370\ \mathrm{cm}^{-1}) \quad (9)$$

Using equations motioned above, NA and NC can be calculated. The calculated results with an uncertainty less than 5%.

References

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