

Quantitative EPR annealing studies of the vacancy-hydrogen complex in single crystal CVD diamond

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Recently attention has been focused on the structure and properties of vacancy-hydrogen and vacancy-nitrogen-hydrogen complexes in diamond detected by Electron Paramagnetic Resonance (EPR) [1,2]. Both these complexes have only been observed in diamond produced by chemical vapour deposition (CVD) and to date nothing is known about the stability of these defects. Here we report the results of isothermal and isochronal EPR annealing studies of the vacancy-hydrogen complex.

Studies such as this require quantitative EPR concentration measurements. Many error sources influence the accuracy and reproducibility of quantitative EPR spectroscopy and we will report on how these have been reduced. To minimise the errors associated with double integration, base line correction, the limits of integration etc, especially in cases where we have overlapping EPR spectra, we have developed spectrum fitting software (using a simplex algorithm) which can account for different lineshapes and the effects of field modulation. Given the line positions and relative intensities of the EPR systems present, the software optimises a lineshape function, derived from the Tsallis distribution, independently for each system (or indeed each line), to produce the best fit to the experimental spectrum. The fit is then used to determine the double integrated intensity and hence concentration of each species present. Howarth and co-workers [3] showed that the Tsallis distribution often provides a better approximation of the experimental spectrum, and generalizes to the Gaussian and Lorentzian lineshapes at the appropriate limits. The simulation software correctly accounts for the field modulation using pseudo-modulation [4], enabling modulation amplitude lineshape distortions to be accounted for in the fitting process. This is important because to obtain good a signal to noise ratio it is often necessary to "over-modulate".

Examples of the usefulness of the fitting software will be presented, and it will be shown that the errors in quantitative EPR can be reduced to a few percent. Finally, it will be shown that the vacancy-hydrogen centre in diamond anneals out with an activation energy of 4.3 ± 0.2 eV and the significance of this result discussed.

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References

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