

Electrical characterisation of defects in polycrystalline B-doped diamond films

O. S. Elsherif^{1, a, *}, K. D. Vernon-Parry^{1, b}, J. H. Evans-Freeman^{2, c},
and P. W. May^{3, d}

¹ Materials and Engineering Research Institute, Sheffield Hallam University, S1 1WB, UK

² College of Engineering, University of Canterbury, Christchurch, New Zealand

³ School of Chemistry, University of Bristol, Bristol, BS8 1TS, UK

^aOsama.S.El-sherif@student.shu.ac.uk, ^bK.Vernon-Parry@shu.ac.uk,

^cjan.evans-freeman@canterbury.ac.nz, ^dpaul.may@bristol.ac.uk

Keywords: Polycrystalline diamond, point and extended defects, DLTS, admittance spectroscopy

Abstract. Admittance spectroscopy (AS) and deep level transient spectroscopy (DLTS) have been applied to B-doped thin polycrystalline diamond films deposited on p⁺-silicon by hot filament chemical vapour deposition. Films with two boron concentrations ($1.5 \times 10^{19} \text{ cm}^{-3}$ and $4 \times 10^{19} \text{ cm}^{-3}$) were selected to study the effect of B concentration on the electronic states in CVD-diamond. We have investigated whether these deep states arise from point or extended defects. DLTS and AS find two hole traps, E1 ($0.29 \pm 0.03 \text{ eV}$) and E2 ($0.53 \pm 0.07 \text{ eV}$), in both films. A third level, E3 ($0.36 \pm 0.02 \text{ eV}$) was also detected in the more highly doped film. The defect levels E1 and E2 exhibited behaviour typical of extended defects, which we suggest may be due to B segregated to the grain boundaries. In contrast, the defect level E3 exhibited behaviour characteristic of an isolated point defect, which we attribute to B-related centres in bulk diamond.

Introduction

Boron is known as the most effective acceptor in diamond for use in electronic devices [1] despite the dopant ionization energies, especially in polycrystalline diamond, being higher than ideal at about 0.36-0.37 eV. However, more than ten percent of the boron atoms incorporated into diamond do not act as acceptors [2]. In polycrystalline diamond, B segregates into highly defective regions of the material such as grain boundaries, and may be trapped there as electrically inactive complexes. The electronic properties of polycrystalline diamond are affected by defects and impurities introduced during the growth and subsequent processing steps during device fabrication. Although high quality material has already been demonstrated [1,3,4], a deeper and more thorough understanding of the physics of defects in polycrystalline diamond is still required for device applications.

Deep level transient spectroscopy (DLTS) [5] and admittance spectroscopy (AS) are powerful techniques for investigating the electronic behaviour of deep levels in semiconductors [6]. AS is slightly less sensitive than DLTS because the deep-level response is probed only by a small region, not by the whole space-charge region as in DLTS. However, electric field effects on the ionization energy are more easily controlled during AS [6]. Recently valuable information about defects in monocrystalline [3] and polycrystalline [7] diamond films have been obtained using DLTS; however, the precise origins of these traps have still not been confirmed.

In this work, a comparison of electrically active defects in polycrystalline CVD diamond containing different boron contents was carried out. DLTS was used to detect deep electronic states and to determine whether they originated from point or extended defects. AS also detected deep levels and gave accurate capture cross section (σ_p) extrapolation for traps associated with extended defects which is not possible using DLTS. Finally, results from AS and DLTS have been compared for semiconducting diamond to confirm that these two techniques yield comparable data.

Experimental method

Boron-doped polycrystalline diamond films, 4 μm thick, were deposited on p^+Si substrates by hot filament CVD (HFCVD). The gas mixture used was high purity H_2 (200 sccm), CH_4 (2 sccm) and diborane (B_2H_6) as the variable source of boron. An estimation of the B content was made for each film by comparison with a calibration graph of 4-point probe resistivity measurements against B content measured by SIMS [4]. The B concentration in these samples was estimated to be $1.5 \times 10^{19} \text{ cm}^{-3}$ in sample 1 and $4 \times 10^{19} \text{ cm}^{-3}$ in sample 2. The diamond films were degreased then immersed in a saturated solution of H_2SO_4 and HNO_3 acid at around 200°C for 20 min to remove graphitic layers and to O-terminate the surface. Films were subsequently annealed in vacuum at 750°C for 30 minutes. 1 mm diameter circular Schottky contacts were formed on the oxidized surface using thermally evaporated Al dots. Al Ohmic contacts were evaporated on the Si back surface. The DLTS and AS measurements were performed using a closed-cycle He high-stability cryostat.

Results and discussion

Schottky diode parameters were investigated in the 200 – 450 K temperature range (at $\pm 5 \text{ V}$); the ideality factor was 1.2 and 2 and the barrier height was about 1.5 and 1.3 eV (at 450 K) for samples 1 and 2, respectively, in agreement with values previously reported [8].

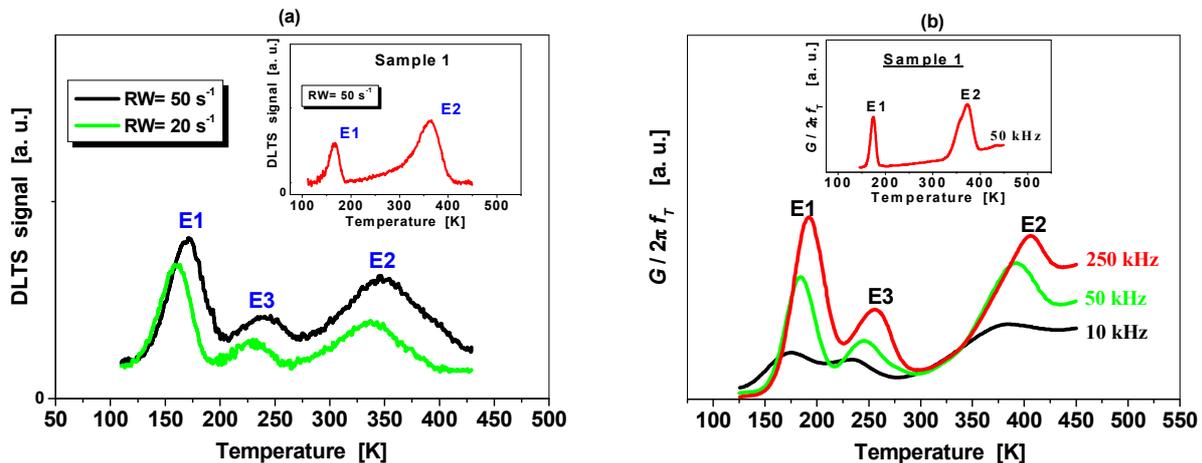


Figure 1. (a) DLTS spectra of sample 2, measured at reverse bias -3 V and fill pulse -0.5 V . Inset shows sample 1 using same biasing conditions and a rate window (RW) 50 s^{-1} . (b) Admittance spectroscopy spectra of sample 2. The inset shows AS spectrum of sample 1, measured at 50 kHz and a reverse bias -3 V .

Fig. 1(a) shows DLTS spectra for sample 2, the inset shows a DLTS spectrum for sample 1. Two majority carrier traps were revealed in the DLTS spectrum of sample 1; Trap E1 was around 170 K with an activation energy (E_a) $0.29 \pm 0.03 \text{ eV}$, and the second peak (E2) covered a wide range of temperatures from 320 K to 440 K with $E_a = 0.53 \pm 0.07 \text{ eV}$. Both peaks shift towards higher temperatures for higher rate windows (RW) as expected. The peaks are asymmetric with a tail on the low-temperature side, a feature typical of an extended defect, but not definite proof of the same. Kiyota *et al.* [9] reported a trap with $E_a = 0.6 \text{ eV}$ in B-doped polycrystalline diamond films grown on Si that they attributed to grain boundaries.

DLTS spectra of sample 2 show both E1 and E2 and a new peak (E3), centred around 250 K, with an $E_a = 0.35 \pm 0.07 \text{ eV}$. A defect with similar E_a has been reported in B-doped diamond, grown by HFCVD, detected by AS in the 170-260 K temperature range; the origin of this level has not been confirmed [10].

AS experiments were carried out on both samples at reverse bias of 0 V and -3 V . Fig. 1(b) shows the AS spectra recorded at -3 V and different probing frequency (f_T) values (10, 50 and 250 kHz) where G is the measured conductance. The frequency peaks shift towards higher temperatures

with increasing f_T , indicating an increase in hole-emission rate. The G/ω peaks occurring at each temperature were used to construct an Arrhenius plot, and hence deduce E_a and the apparent capture cross-section (σ_p) of each defect, at zero bias, according to the standard equation [6]:

$$\frac{2\pi \cdot f_T}{T_{max}^2} = \sqrt{96 \pi^3} \cdot g \cdot \frac{m^* k^2}{h^3} \cdot \sigma_p \cdot \exp\left(\frac{-E_a}{k T_{max}}\right) \quad (1)$$

where T_{max} is the temperature of the conductance peak, m^* is the effective mass of the hole, h is Planck's constant, k is the Boltzmann constant, and g is the degeneracy factor.

The G/ω vs. T data qualitatively reproduce the behaviour observed in the DLTS experiments, and the activation energies of the trap levels determined by AS are in close agreement with those calculated from DLTS, see Table 1. It should be noted that electric field effects on the ionization energy are more controlled in AS than conventional DLTS [6].

Table 1. Summary of the deep levels calculated by DLTS and AS.

Trap	N_T [cm ⁻³]	$E_T - E_V$ [eV]		σ_p [cm ²]	
		DLTS	AS	DLTS	AS*
E1	5×10^{16}	0.29 ± 0.03	0.26 ± 0.04	n/a	2×10^{-18}
E2	7×10^{16}	0.53 ± 0.07	0.58 ± 0.03	n/a	8×10^{-19}
E3	3×10^{16}	0.35 ± 0.02	0.36 ± 0.02	3×10^{-15}	2×10^{-15}

* Measured at 0 V.

n/a Values cannot be determined by DLTS because Eq. 2 does not have a linear fit.

N_T Trap concentration calculated from DLTS.

Fig. 2(a) shows the capacitance change as a function of the fill-pulse length (t_p) in DLTS, in accordance with Eq. 2 [5].

$$\ln \left[\frac{\Delta C_\infty - \Delta C_t}{\Delta C_\infty} \right] = \sigma_p \cdot v_{th} \cdot p \cdot t_p \quad (2)$$

where ΔC_∞ is the equilibrium capacitance value, ΔC_t is the capacitance at time t , p is the majority carrier population, and v_{th} is the thermal velocity.

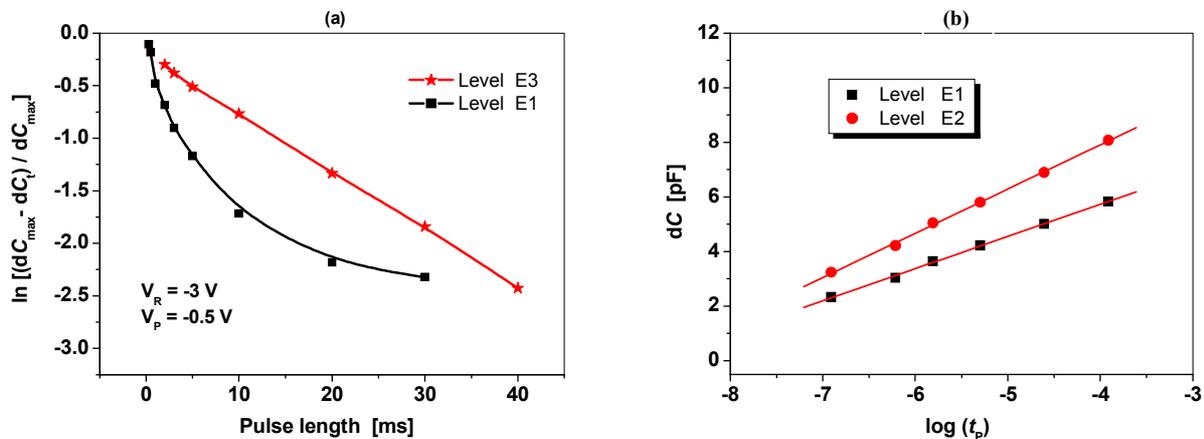


Figure 2. (a) The capacitance change as a function of t_p for E1 in sample 1 and E3 in sample 2, measured at 170 K and 250 K respectively. (b) The DLTS signal amplitude as a function of the logarithm of the filling time for the defects at E1 and E2 in sample 1, measured at 170 K and 360 K respectively, at $V_R = -3 V$ and fill pulse $-0.5 V$.

The capture cross-section should obey a linear dependence on the logarithm of a combination of capacitance terms as function of t_p . Deviation from this relationship provides a sensitive test for the presence of extended defects that exhibit Coulombic repulsion. This is the case for the defects causing levels E1 and E2. It is known that the DLTS signal should exhibit a dependence on $\log(t_p)$ when the carrier capture is into extended defects [11],

$$\Delta C_m \propto \ln(t_p) \quad (3)$$

where ΔC_m denotes the amplitude of the DLTS signal.

Fig. 2(b) shows the data for levels E1 and E2 in sample 1 plotted in accordance with Eq. 3. An excellent fit was obtained, confirming that the defects giving rise to this capture characteristic are extended states.

Summary

Deep trap levels in boron-doped diamond have been investigated experimentally using DLTS and AS, as a function of doping concentration. Data recorded by DLTS and AS yielded identical information about the deep levels in CVD-diamond films; identified by DLTS as hole traps. Levels E1 and E2 were found in both films; level E3 was found in the more highly doped film only.

The DLTS analysis of levels E1 and E2 demonstrated that the trapping is at extended defects, possibly B segregated at grain boundaries in these films. The electrical behaviour of the defect responsible for level E3 suggests that this trap consists of isolated point defects, which, taken with the fact that it is not found in the less heavily doped film, is consistent with it being associated with a B-related centre in bulk diamond.

References

- [1] R. Kalish: *Int. J. Nanotechnol.* 6 (2009) 691-703
- [2] J. Chevallier, B. Theys, A. Lusson, C. Grattelain, A. Deneuville and E. Gheeraert: *Phys. Rev. B* 58 (1998) 7966-7969
- [3] P. Muret, J. Pernot, A. Kumar, L. Magaud, C. Mer-Calfati and P. Bergonzo: *Phys. Rev. B* 81 (2010) 235205
- [4] P. W. May, W. Ludlow, M. Hannaway, P. Heard, J. Smith and K. Rosser: *Diamond & Related Materials* 17 (2008) 105-117
- [5] D. V. Lang: *J. Appl. Phys.* 45 (1974) 3023-3032
- [6] J.L. Paustrat, B. Katircioglu, N. Magnea, D. Bensahel, J.C. Pfister and L. Revoil: *Solid-State Electron.* 23 (1980) 1159-1169
- [7] V.I. Polyakov, A.I. Rukovishnikov, L.A. Avdeeva, Z.E. Kun'kova, V.P. Varnin, I.G. Teremetskaya and V.G. Ralchenko: *Diamond & Related Materials* 15 (2006) 1972-1975
- [8] D. A. Evans, O. R. Roberts, G. T. Williams, A. R. Vearey-Roberts, F. Bain, S. Evans, D. P. Langstaff and D. J. Twitchen: *J. Phys.: Condens. Matter* 21 (2009) 364223
- [9] H. Kiyota, H. Okushi, K. Okano, Y. Akiba, T. Kurosu and M. Iida: *Appl. Phys. Lett.* 61 (1992) 1808-1810
- [10] Adenilson J. Chiquito, Olívia M. Berengue, Edgar Diagonel, José C. Galzerani and João R. Moro: *J. Appl. Phys.* 101 (2007) 033714
- [11] P. N. Grillo, S. A. Ringel, E. A. Fitzgerald, G. P. Watson and Y. H. Xie: *J. Appl. Phys.* 77 (1995) 676-685

Silicon Carbide and Related Materials 2011

10.4028/www.scientific.net/MSF.717-720

Electrical Characterisation of Defects in Polycrystalline B-Doped Diamond Films

10.4028/www.scientific.net/MSF.717-720.1315