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2007 J. Phys.: Condens. Matter 19 306204

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J. Phys.: Condens. Matter **19** (2007) 306204 (6pp) doi:10.1088/0953-8984/19/30/306204

Thermal stability of defects in p-type as-grown 6H-SiC

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Received 2 March 2007, in final form 15 June 2007
Published 11 July 2007
Online at stacks.iop.org/JPhysCM/19/306204

Abstract
An isochronal annealing series was performed in order to investigate the thermal behaviour of as-grown defects in Al-doped 6H-SiC. Five hole traps have been detected, by means of deep level transient spectroscopy (DLTS), above the valence band (E_V) in the 0.2–1.3 eV energy range. One trap, labelled MZ2, anneals out after a 1800 °C heat treatment, while the others display higher thermal stability. The nature of these centres is discussed on the basis of the previous experimental and theoretical data found in the literature. Particular emphasis has been given to a trap labelled MZ3, which we identified as the D-centre, and to the effect that the electric field has on its emission time constant.

1. Introduction

As a consequence of the improvement in growth techniques, silicon carbide (SiC) is now considered as the best candidate for replacement of silicon (Si) in a large number of electronic applications. Its chemical inertness as well as its extraordinary electrical properties make SiC the first choice semiconductor for devices working in harsh environments. However, the presence of both impurities and intrinsic/extrinsic defects may give rise to electrically active centres in the bandgap. These centres may behave as recombination centres or can act as traps for electron or holes, limiting the lifetime of charge carries. It is therefore technologically relevant to study such levels, because it is crucial to bear in mind knowledge of their electrical properties, thermal behaviour and microscopic structure when designing electronic devices.

A large number of both theoretical [1, 2] and experimental [3–5] studies on the thermal stability and nature of intrinsic defects of n-type SiC polytypes can be found in the literature. As an example, the atomic structure of both the $Z_{1/2}$ and $EH_{6/7}$ defects on 4H-SiC [3] is still an open question and this has attracted the attention of many scientists. However, this has driven attention away from other equally interesting topics, like the thermal stability and nature of intrinsic defects in p-type polytypes. Furthermore, the determination of the charge state of the D-centre is still a matter of discussion. It is now generally accepted that this centre is boron related and that it has a high thermal stability. However, the field dependence of its emission time constant (or emission rate) is not clear. Anikin *et al* [6], who first noticed an enhancement

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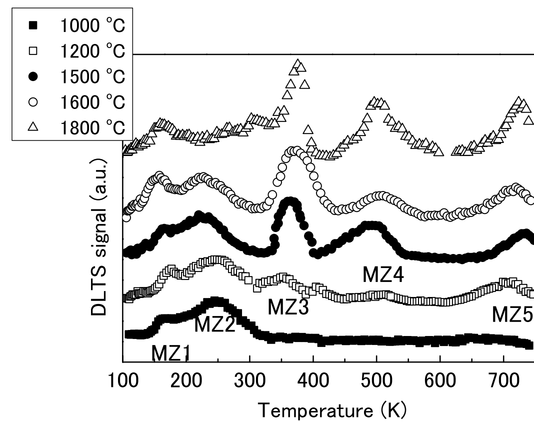

Figure 1. DLTS spectra of p-type 6H-SiC epitaxial layers annealed at 1000, 1200, 1500, 1600 and 1800 °C.

of the emission rate for increasing electric field, talk of the acceptor nature of the D-centre, while Suttrop *et al* [7], have found that indeed high electric fields cause an enhancement of the emission rate, but such enhancement is too low in comparison with what the Poole–Frenkel theory predicts.

Recently, Negoro *et al* [8] performed a capacitance–voltage (C–V) study on B-implanted 4H-SiC and concluded that the concentration of the shallow B acceptor could only be explained by assuming that the D-centre was neutral after hole capture. However, to our knowledge the charge state of the D-centre has not yet been fully clarified. In our contribution, we carried out an isochronal annealing study in the 1000–1800 °C temperature range, performing deep level transient spectroscopy (DLTS) measurements after each annealing step. We detected five traps and studied their annealing behaviour, comparing our results with those reported by other authors. Furthermore, one of these traps was identified as the D-centre and we discussed the decrease of its emission time constant (increase of its emission rate) for increasing electric field, in detail, in the light of theoretical predictions.

2. Experimental details

An isochronal annealing series, in the temperature range 1000–1800 °C, with a time constant of 15 min, and performed in Ar ambient, was carried out on Al-doped ($N_a - N_d = 8 \times 10^{15}$ cm^{-3}) 6H-SiC epitaxial layers grown by chemical vapour deposition (CVD) and purchased from CREE. After every annealing step, first Ti/Al/Ni Ohmic contacts (sintered at 1000 °C by rapid thermal annealing) and then Ti Schottky diodes (diameter 500 μm) were formed by thermal evaporation. Samples were electrically characterized by means of Fourier DLTS [9], in the 100–750 K temperature range, with a reverse bias of 5 V and an applied bias of 0 V. Note that the net acceptor concentration was unchanged in these annealing experiments.

3. Results and discussion

3.1. Isochronal annealing study

In figure 1 the results of the DLTS measurements after thermal treatments at 1000, 1200, 1500, 1600 and 1800 °C are shown. We detected five hole traps in the 0.22–1.3 eV energy range,

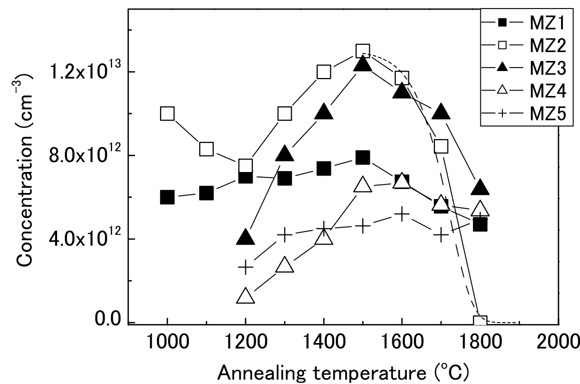

Figure 2. Isochronal annealing behaviour (time constant = 15 min) of the five detected levels. The dashed curve represents a first order dissociation process with an activation energy of 6.4 eV and pre-exponential factor of 10^{13} s^{-1}.

above the valence band E_V. After annealing for 15 min at 1000 °C we found two levels, MZ1 and MZ2 respectively. According to the few data found in the literature it is possible to identify the MZ1 centre with the boron acceptor, since its temperature and energy position agrees well with what has been reported by other authors [7]. On the other hand, no reports of the MZ2 level exist in the literature, therefore no concrete hypothesis on the atomic nature of the detected levels can be put forward yet. Only by performing annealing treatments at higher temperatures (1200 °C) were we able to detect the other three traps: MZ3 and MZ5 are clearly distinguishable, while MZ4 is also present but at a very small concentration. By further heat treatments at 1500 and 1600 °C, the MZ4 DLTS peak becomes clearly visible and it can also be noted that the width of both MZ2 and MZ4 is around 100 K, suggesting that they may be due to the overlapping of minor contributions. MZ3 is very close to the energy level assigned to the D-centre [7], while the MZ4 level has a very similar band gap position to the Hp1 level ($E_V + 0.66$ eV) detected by Storasta *et al* [11]. To our knowledge this is also the first report of the MZ5 centre which may be identified as the HK3 ($E_V + 1.27$ eV) [10] counterpart in 6H-SiC. Although the studies cited in [10, 11] were performed on the 4H polytype, the energy level positions in the band gaps are comparable due to the alignment of the valence bands of the 4H and 6H polytypes [12]. After performing a heat treatment at 1800 °C, the MZ2 centre anneals out while all the other traps still persist.

Obviously, due to the lack of reports in the literature and to the limited amount of experimental data, more work is needed to reach a conclusive identification of these levels, even though it is well established that the D-centre is a complex involving boron (either B_{Si}–V_C or B_C–V_C [13]). However, from the isochronal annealing behaviour of the traps, it is possible to extract some useful hints.

Figure 2 shows the detailed isochronal annealing behaviour of all the detected traps. It can be seen that while MZ2, MZ3 and MZ4 display a significant variation in concentration, MZ1 and MZ5 do not show meaningful changes. The concentration of MZ2 decreases slightly in the 1000–1200 °C temperature range, increasing up to 1500 °C and then annealing out. This annealing behaviour is similar to what is observed for the $Z_{1/2}$ centre after high energy electron irradiation [5], and may indicate that the nature of the MZ2 centre is likely to be related to a complex structure. Moreover, in an analogous manner to what is described in [5], we can obtain, from the annealing behaviour of MZ2, an activation energy for a first order

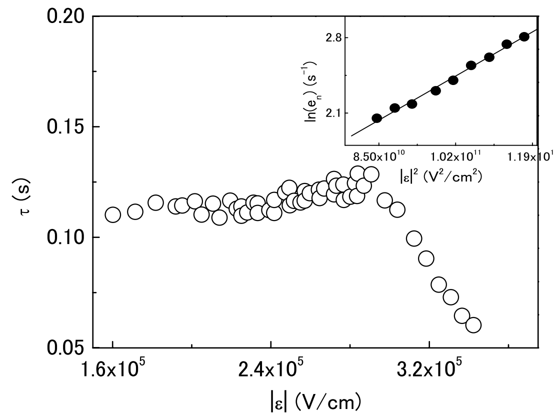

Figure 3. Electric field dependence of the emission time constant. The inset shows the linear fit for the logarithm of the emission rate versus the squared field.

Table 1. Labelling, energy position in the band gap above E_V and possible identification for the five detected traps. The values of the energies are affected by some error due to the relatively small DLTS signals.

Label	Energy (eV)	Comments
MZ1	0.2–0.3	B-acceptor?
MZ2	0.3–0.4	Complex?
MZ3	0.55 ± 0.02	D centre
MZ4	0.64 ± 0.05	Hp1
MZ5	1.30 ± 0.04	HK3

dissociative process of 6.4 eV (dashed curve in figure 2). Labelling, energy position and possible identification of the five detected traps are reported in table 1.

3.2. Field dependence of the emission time constant of the D-centre

As previously mentioned, Suttrop *et al* [7] observed a slight increase in the emission rate of the D-centre for electric field strengths ($|\vec{\varepsilon}|$) higher than 150 kV cm^{-1}, but such enhancement was lower than that of a Coulombic centre with charge state 1. This disagrees with previous experimental studies [6]. As can be seen in figure 3, we measured the variation of the emission time constant (τ) for electric field strength varying from 150 up to 350 kV cm^{-1} and found a decrease of τ for $|\vec{\varepsilon}|$ higher than 280 kV cm^{-1}. Following the theoretical studies by Vincent *et al* [14], the electric field dependence of the emission time constant can be described by different models according to the magnitude of $\vec{\varepsilon}$. Since τ decreases in the 10^5 V cm^{-1} range, the pure tunnelling effect can be ruled out as a possible explanation. On the other hand, for our range of magnitudes two other models can apply: the Poole–Frenkel and phonon-assisted tunnelling ones.

Although it is known that the Poole–Frenkel model is in general dominant for the lower fields (10^4 V cm^{-1}) [14] we applied the criterion suggested by Ganichev *et al* [15], which is a simple and effective way to determine which of the two models can best describe a set of data. This criterion simply consists of fitting the logarithm of the emission rate versus the squared electric field with a straight line. As shown in the inset of figure 3, we also applied such a criterion and found that the logarithm of the emission rates versus the squared electric field

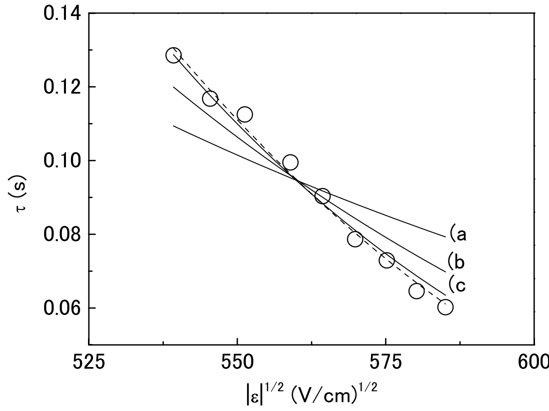

Figure 4. Variation of the emission time constant, fitted with (a) Coulomb, (b) Dirac and (c) square-well potential. The dashed curve refers to a semiclassical phonon-assisted tunnelling model.

can be fitted linearly, indicating that our data can be described by a phonon-assisted tunnelling model [15].

On the basis of such preliminary results, we tried to describe the observed lowering of the emission barrier by using the analytical expression of the Poole–Frenkel effect, as derived by Hartke [16] (for a Coulomb, Dirac [14] and square-well [17] potential) and for the phonon-assisted tunnelling mechanism.

The Coulomb potential was our first choice

$$\begin{aligned} \tau_0/\tau &= (\mathrm{e}^{\gamma}(\gamma - 1) + 1)/\gamma^2 + 1/2 \\ \gamma &= (nq|\vec{\varepsilon}|/\pi\epsilon\epsilon_0)^{1/2} q/k_\mathrm{B}T \end{aligned} \qquad (1)$$

with τ_0 the zero-field emission time constant, n the charge state, q the electronic charge, ϵ_0 the permittivity in the free space, ϵ the permittivity in the host crystal, k_B the Boltzmann constant and T the temperature. It can be seen in figure 4 that our data cannot be explained either by using this model, with τ_0 as a free parameter and $n = 1$ (solid line (a)), or by using a Dirac potential well (solid line (b), charge state $n = 2$). On the contrary a good fit can be obtained by employing a square well potential:

$$\begin{aligned} \tau_0/\tau &= (\mathrm{e}^{\gamma} - 1)/2\gamma + 1/2 \\ \gamma &= nq|\vec{\varepsilon}|r_0/k_\mathrm{B}T. \end{aligned} \qquad (2)$$

with τ_0 and radius r_0 as free parameters. A value of 4.95 nm for r_0 (solid line (c), charge state $n = 1$) was obtained, corresponding to a cross section of about 8×10^{-15} cm^2, which agrees reasonably well with the capture cross section of the D-centre [7]. Furthermore, we also applied the semiclassical phonon-assisted tunnelling model by Karpus and Perel [18] (dashed line) and found that it can describe our experimental data quite well. Very small differences can be noticed between the square well potential and phonon-assisted tunnelling models because the former gives good phonon-assisted tunnelling rates [17]. For this reason, it is difficult to establish which of the two models is more suitable for describing our set of data.

4. Conclusions

We investigated the thermal stability of five detected levels in p-type 6H-SiC by means of DLTS. An isothermal annealing series was performed and revealed that while all the centres

display a high thermal stability, only one labelled MZ2 was annealed out after heat treatments at 1800 °C. An activation energy for a first order dissociative process of 6.4 eV was estimated and this value was compared with what has been reported in the literature. The MZ3 level was identified as the D-centre, and the field dependence of its emission time constant revealed that such a dependence could be described by either employing a 4.95 nm square well potential or by a phonon-assisted tunnelling process.

Acknowledgment

Financial support by the Japanese Society for the Promotion of Science (JSPS) is gratefully acknowledged.

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