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Original Publication:

Franziska Beyer, Carl Hemmingsson, Andreas Gällström, Stefano Leone, Henrik Pedersen, Anne Henry and Erik Janzén, Deep levels in tungsten doped n-type 3C-SiC, 2011, APPLIED PHYSICS LETTERS, (98), 15, 152104.
http://dx.doi.org/10.1063/1.3579527

Deep levels in tungsten doped n-type 3C–SiC

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(Received 1 March 2011; accepted 25 March 2011; published online 13 April 2011)

Tungsten was incorporated in SiC and W related defects were investigated using deep level transient spectroscopy. In agreement with literature, two levels related to W were detected in 4H–SiC, whereas only the deeper level was observed in 6H–SiC. The predicted energy level for W in 3C–SiC was observed ($E_C-0.47$ eV). Tungsten serves as a common reference level in SiC. The detected intrinsic levels align as well: E1 ($E_C-0.57$ eV) in 3C–SiC is proposed to have the same origin, likely V_C, as EH6/7 in 4H–SiC and E7 in 6H–SiC, respectively. © *2011 American Institute of Physics*. [doi:10.1063/1.3579527]

In recent years, much progress has been achieved in identifying the minority carrier lifetime limiting defects in SiC and it has been shown that thermal oxidation[1,2] and carbon-implantation/annealing[3] resulted in increased lifetimes and a large reduction in the intrinsic levels $Z_{1/2}$ and EH6/7 in 4H–SiC. Most investigations were conducted on the 4H–SiC polytype and only recently, a comparative study on defects in 4H–SiC and 6H–SiC and their behavior after oxidation has revealed common characteristics on the origin of these intrinsic defects.[4] Previously, defect studies on 3C–SiC bulk material[5] and cubic layers grown on Si have been done.[6–9] However, due to the heteroepitaxial growth, it has not been clear, which of the defects are related to the interface and which that are related to 3C–SiC. Chloride-based chemical vapor deposition (CVD) of cubic SiC on hexagonal on-axis SiC has been shown to produce high quality materials[10] and defect studies in such materials[11] may guide to a common view on the deep levels and their origin in SiC.

Defect identification using electrical characterization techniques alone, such as deep level transient spectroscopy (DLTS) is difficult; additional characterization techniques, such as electron spin resonance or photoluminescence, are usually required. The implantation of known radioactive elements avoid such problems.[12] V and Cr as well as Ti and other metals have been identified in SiC using this technique. In previous studies on electrical characterization of tungsten (W) in SiC, the transition metal was introduced either by implantation of radioactive ^{178}W in 4H–SiC, 6H–SiC, and 15R–SiC (Refs. 13 and 14) to investigate the decay to daughter isotopes or by unintentional introduction of W in 6H–SiC due to contamination from the growth reactor.[15,16]

In this paper, we study the transition metal W in the SiC polytypes 4H, 6H, and 3C by DLTS to confirm experimentally the previously calculated energy level for W in 3C–SiC. Comparison between the different polytypes suggests that the valence band is pinned to the same level[17] in 4H–SiC, 6H–SiC, and 3C–SiC assuming W is following the *Langer Heinrich rule*.[18]

The different SiC epilayers were grown using a chloride-based CVD process[19] on highly doped off-axis substrates (6H–SiC) or in the case of the reference 3C–SiC sample on a semi-insulating on-axis substrate (4H–SiC). The epilayers were intentionally contaminated with W by placing small metallic flakes (2×2 mm^2) directly on the substrate and in the upstream part of the susceptor. Metallic contacts were thermally evaporated onto the epilayers after chemical cleaning and etching of the native oxide by hydrofluoric acid. For the 3C layers an additional preparative step was introduced to saturate surface states by oxidation.[20] UV-illumination from an Argon ion laser formed the oxidizing environment at an elevated temperature ($T=200$ °C). Thick circular Ni contacts (about 1000 Å) served as rectifying contacts for the 4H–SiC and 6H–SiC epilayers, whereas the Ohmic contact was achieved using conducting silver paint to the highly doped substrate. In case of 3C-epilayers, both rectifying (Au, about 2500 Å) and Ohmic (Al, 2000 Å) contacts were deposited onto the epitaxial surface. The rectifying behavior was checked by current-voltage (IV) measurements and a homogenous doping distribution was confirmed by capacitance voltage (CV) measurements at room temperature. The net doping concentration, N_d-N_a varied for the different polytypes depending on the growth conditions but also whether the sample was doped with W or not. The deep levels were investigated using DLTS in a temperature range from 85 to 700 K. The following DLTS parameters were used for the 4H- and 6H-samples: filling pulse length of 10 ms and a filling pulse height of 10 V. The quiescent reverse bias was $V_r=-10$ V. Due to inferior IV characteristics a reverse bias of only 2 V was used for the 3C-layers. The filling pulse height was 1.5 V with a pulse length of 10 ms. The capacitance transients were evaluated using conventional boxcar technique or, in the case of the 3C-layers by lock-in amplification simulation to reduce the noise level.

Figure 1 displays the DLTS spectra of the different polytypes doped with W: 4H–SiC (squares), 6H–SiC (stars), and 3C–SiC (triangles). In the as-grown material, we observe only intrinsic defects, such as $Z_{1/2}$ and EH6/7 in 4H–SiC, E1/2 and E7 in 6H–SiC, and E1 in 3C–SiC, respectively. The spectrum of 4H–SiC clearly shows additional peaks besides the well-known intrinsic levels $Z_{1/2}$ and EH6/7. As reported by Achtziger,[14] W has one shallow ($E_A=E_C-0.17$ eV) and one deep ($E_A=E_C-1.43$ eV) level in 4H–SiC. Both levels were detected in our epitaxial layers. The electronic properties for these levels are summarized in Table I. For the shallower tungsten peak, labeled W1, the capture cross section was determined using different filling pulse lengths

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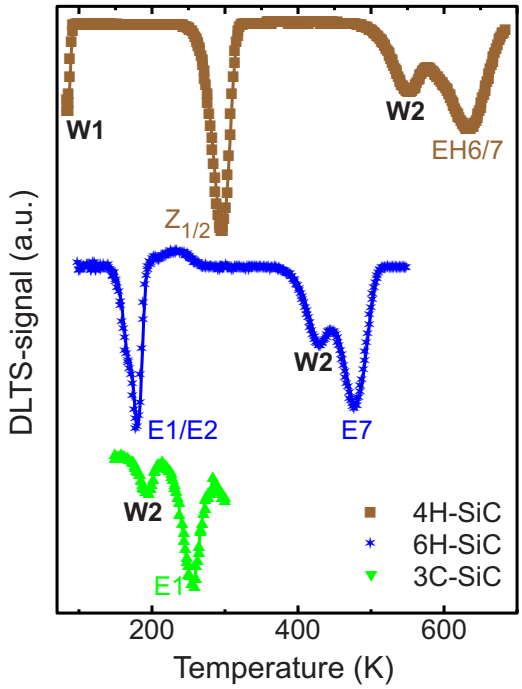

FIG. 1. (Color online) DLTS spectra of the W doped SiC samples; 4H–SiC (squares): rate window (13.9 s)$^{-1}$; 6H–SiC (stars): rate window (2.8 s)$^{-1}$; DLTS parameters: t_p=10 ms, V_r=−10 V, and V_p=10 V and 3C–SiC (triangles): rate window (4.7 s)$^{-1}$; DLTS parameters: t_p=10 ms, V_r=−2 V and V_p=1.5 V.

(t_p=50 ns−1 s) to $\sigma_{meas}=(5.9\pm0.8)\times10^{-15}$ cm^2. In Ref. 14 the capture cross section was estimated to be larger than 2×10^{-16} cm^2 in agreement with our results. For the deeper tungsten level, W2, the capture cross section was determined to $\sigma_{meas}=(1.1\pm0.5)\times10^{-14}$ cm^2 (t_p=50 ns−20 μs). The capture cross section obtained for the EH6/7 level of $\sigma_{meas}(EH6/7)=(5.3\pm0.1)\times10^{-15}$ cm^2 agrees with the previously reported values by Hemmingsson *et al.*[21] The σ_{meas} of the W2 and EH6/7 did not change in a temperature window of 30 K, whereas the capture cross section of the $Z_{1/2}$-level showed a clear temperature dependence.[22]

The DLTS spectrum of 6H–SiC intentionally doped with W is also shown in Fig. 1, (stars). The previously reported W related peak[14,16] at $E_A=E_C-1.16$ eV was observed in our doped samples, labeled W2. The electrical properties can be found in Table I. The capture cross sections of the W2- and the E7-levels were $\sigma_{meas}(W2)=(8.8\pm0.7)\times10^{-15}$ cm^2 and $\sigma_{meas}(E7)=(9.1\pm0.6)\times10^{-15}$ cm^2, respectively (t_p=50 ns−20 μs). Hemmingsson *et al.*[24] reported similar value for the capture cross section of the E7-level. In a range of ΔT=66 K, σ_{meas} stayed constant for the W2 peak and for the E7, whereas it varied for the E1/E2-level[23,24] similar to the behavior of the $Z_{1/2}$-level in 4H–SiC. Assuming the valence band is pinned to the same level in different polytypes,[17,25] the shallower level W1, which was detected in 4H–SiC, should be located in the conduction band for the 6H polytype. Additionally, studies on semiconductor heterojunctions showed that deep levels related to transition metals serve as *common reference levels* in isovalent semiconductor compounds, known as *Langer–Heinrich rule*.[18] In Ref. 26, the authors presented W related states in 4H–SC, 6H–SiC, and 15R–SiC together with calculations on 3C–SiC. The authors confirm experimentally the valence band edge alignment and that defects related to the transition metals, Ta and W, are common reference levels in SiC. Furthermore, they strengthen their arguments by prediction on the position of the W level in 3C–SiC.

Figure 1 (triangles) shows a DLTS spectrum of our grown 3C–SiC doped with W. We observe two peaks in the spectrum, labeled W2 and E1. The determined activation energy of W2 ($E_A=E_C-0.47$ eV, see Table I) agrees well with the calculated double donor level at $E_A=E_V+1.94$ eV (Ref. 26) assuming a bandgap of E_g=2.36 eV at room temperature.[27] The other peak, E1 is close to the W6-level observed in irradiated 3C–SiC,[28] in hydrogen implanted 3C–SiC,[29] and in as-grown heteroepitaxial grown 3C–SiC.[11] The authors therein relate the electron trap to an intrinsic defect similar to $Z_{1/2}$ or EH6/7 in 4H–SiC.

Comparing the different polytypes, see Fig. 1, the deep tungsten level, W2, is observed at lower temperatures than the EH6/7 in 4H–SiC and the E7 in 6H–SiC, respectively. The shape of the two peaks is very similar for all polytypes. Sasaki *et al.*[4] recently showed that these levels most probably originate from the same defect, likely the carbon vacancy. They additionally concluded that the *Langer–Heinrich rule*, which was previously only applied for transition metals, is valid also for intrinsic defects in SiC. Our results support this suggestion. Also for the 3C–SiC, a level is observed at higher activation energy, the E1. This level was related to the $Z_{1/2}$ in 4H–SiC.[28,29] However, taking the valence-band alignment into account, the level is more related to EH6/7 in 4H–SiC or E7 in 6H–SiC than to the $Z_{1/2}$-level or $E_{1/2}$ in 4H–SiC or 6H–SiC, respectively. Thus the observed E1 in 3C–SiC is likely related to the carbon vacancy as well. In Fig. 2, we summarize our investigations by displaying the energetic positions of the measured levels in the band gap of the different polytypes. The alignment of the W2 level becomes obvious as well as the alignment of the intrinsic levels, EH6/7, E7 and E1 in 4H–SiC, 6H–SiC, and 3C–SiC, respectively.

In the present study, we have detected the deep W2 level in 3C–SiC; its activation energy agrees well with the predicted one and aligns well with the deep W2 levels in 4H–SiC and 6H–SiC. Tungsten can be regarded as a common reference level in SiC. Additionally, the alignment of intrin-

TABLE I. Properties of the W-peaks and intrinsic levels: E_a and σ are obtained from Arrhenius plots [$\ln(e/T^2)$ vs $1000/T$], whereas σ_{meas} from DLTS measurements with different t_p and N_t from the DLTS peak amplitudes.

	Peak	E_a (eV)	σ (cm^2)	σ_{meas} (cm^2)	N_t (cm^{-3})
4H–SiC	W1	$E_C-0.18$	4×10^{-13}	5.9×10^{-15}	$\approx1\times10^{13}$
	$Z_{1/2}$	$E_C-0.66$	2×10^{-14}	[a]	1.9×10^{13}
	W2	$E_C-1.40$	1×10^{-13}	1.1×10^{-14}	1.3×10^{13}
	EH6/7	$E_C-1.53$	2×10^{-14}	5.3×10^{-15}	2.1×10^{13}
6H–SiC	E1	$E_C-0.35$	2×10^{-15}	[b]	2.3×10^{13}
	E2	$E_C-0.43$	4×10^{-14}	[c]	6.7×10^{13}
	W2	$E_C-1.15$	3×10^{-13}	8.8×10^{-15}	3.6×10^{13}
	E7	$E_C-1.27$	1×10^{-13}	9.1×10^{-15}	6.2×10^{13}
3C–SiC	W2	$E_C-0.47$	1×10^{-13}		6.0×10^{13}
	E1	$E_C-0.57$	6×10^{-15}		1.2×10^{14}

[a]Reference 22: Z_1^-: $1.7\times10^{-15}\exp(-0.065/k_BT)$ cm^2, Z_2^-: $1.3\times10^{-15}\exp(-0.080/k_BT)$ cm^2.
[b]Reference 23: $E_1^{-/+}$: $1.1\times10^{-15}\exp(-0.048/k_BT)$ cm^2.
[c]Reference 23: $E_2^{-/+}$: $7.7\times10^{-15}\exp(-0.070/k_BT)$ cm^2.

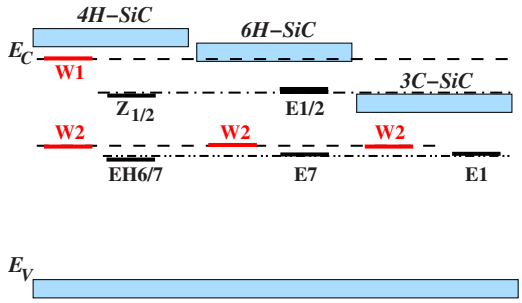

FIG. 2. (Color online) Energetic positions of W related and intrinsic deep levels in the band gap of the various SiC polytypes. Dotted lines are guidelines for the eyes.

sic defect levels was observed, which suggests that the E1 level in 3C–SiC is related to EH6/7 in 4H–SiC and E7 in 6H–SiC, respectively, and thus to the carbon vacancy.

The Swedish Research Council (VR; 2009-3383 and 2008-5243) and the Swedish Energy Agency (P30942-1) are gratefully acknowledged for financial support.

[1]T. Hiyoshi and T. Kimoto, Apex **2**, 041101 (2009).
[2]T. Hiyoshi and T. Kimoto, Apex **2**, 091101 (2009).
[3]L. Storasta, H. Tsuchida, T. Miyazawa, and T. Ohshima, J. Appl. Phys. **103**, 013705 (2008).
[4]S. Sasaki, K. Kawahara, G. Feng, G. Alfieri, and T. Kimoto, J. Appl. Phys. **109**, 013705 (2011).
[5]G. Alfieri and T. Kimoto, Phys. Status Solidi B **246**, 402 (2009).
[6]P. Zhou, M. G. Spencer, G. L. Harris, and K. Fekade, Appl. Phys. Lett. **50**, 1384 (1987).
[7]K. Zekentes, M. Kayiambaki, and G. Constantinidis, Appl. Phys. Lett. **66**, 3015 (1995).
[8]M. Ichimura, Y. Koga, N. Yamada, T. Abe, E. Arai, and Y. Tokuda, Jpn. J. Appl. Phys., Part 2 **37**, L18 (1998).
[9]N. Yamada, M. Kato, M. Ichimura, E. Arai, and Y. Tokuda, Jpn. J. Appl. Phys., Part 2 **38**, L1094 (1999).
[10]S. Leone, F. C. Beyer, A. Henry, O. Kordina, and E. Janzén, Phys. Status Solidi (RRL) **4**, 305 (2010).
[11]F. C. Beyer, S. Leone, C. Hemmingsson, A. Henry, and E. Janzén, AIP Conf. Proc. **1292**, 63 (2010).
[12]N. Achtziger, J. Grillenberger, and W. Witthuhn, Hyperfine Interact. **120-121**, 69 (1999).
[13]N. Achtziger and W. Witthuhn, Appl. Phys. Lett. **71**, 110 (1997).
[14]N. Achtziger, G. Pasold, R. Sielemann, C. Hülsen, H. Grillenberger, and W. Witthuhn, Phys. Rev. B **62**, 12888 (2000).
[15]K. Irmscher, I. Pintilie, L. Pintilie, and D. Schulz, Physica B **308–310**, 730 (2001).
[16]K. Irmscher, Mater. Sci. Eng., B **91–92**, 358 (2002).
[17]V. V. Afanas'ev, M. Bassler, G. Pensl, M. J. Schulz, and E. Stein von Kamienski, J. Appl. Phys. **79**, 3108 (1996).
[18]J. M. Langer and H. Heinrich, Phys. Rev. Lett. **55**, 1414 (1985).
[19]H. Pedersen, S. Leone, A. Henry, V. Darakchieva, P. Carlsson, A. Gällström, and E. Janzén, Phys. Status Solidi (RRL) **2**, 188 (2008).
[20]J. Eriksson, M. H. Weng, F. Roccaforte, F. Giannazzo, S. Leone, and V. Raineri, Appl. Phys. Lett. **95**, 081907 (2009).
[21]C. Hemmingsson, N. T. Son, O. Kordina, J. P. Bergman, E. Janzén, J. L. Lindström, S. Savage, and N. Nordell, J. Appl. Phys. **81**, 6155 (1997).
[22]C. G. Hemmingsson, N. T. Son, A. Ellison, J. Zhang, and E. Janzén, Phys. Rev. B **58**, R10119 (1998).
[23]C. G. Hemmingsson, N. T. Son, and E. Janzén, Appl. Phys. Lett. **74**, 839 (1999).
[24]C. Hemmingsson, N. T. Son, O. Kordina, E. Janzén, and J. L. Lindström, J. Appl. Phys. **84**, 704 (1998).
[25]F. Bechstedt, P. Käckell, A. Zywietz, K. Karch, B. Adolph, K. Tenelsen, and J. Furthmüller, Phys. Status Solidi B **202**, 35 (1997).
[26]J. Grillenberger, N. Achtziger, G. Pasold, R. Sielemann, and W. Witthuhn, Mater. Sci. Forum **353–356**, 475 (2001).
[27]Y. Goldberg, M. Levinshtein, and S. Rumyantsev, *Properties of Advanced Semiconductor Materials: GaN, AlN, SiC, BN, SiC, SiGe* (Wiley, New York, 2001), pp. 93–148.
[28]M. Weidner, G. Pensl, H. Nagasawa, A. Schöner, and T. Ohshima, Mater. Sci. Forum **457–460**, 485 (2004).
[29]M. Weidner, L. Trapaidze, G. Pensl, S. A. Reshanov, A. Schöner, H. Itoh, T. Oshima, and T. Kimoto, Mater. Sci. Forum **645–648**, 439 (2010).