

Identification of carbon-hydrogen complexes in n- and p-type silicon

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The origin of several deep traps E42, E90, E262, and H180 in hydrogenated *n*-type and *p*-type FZ and CZ Si is investigated. Comparing the depth profiles of these defects in samples with different C, O, H, and shallow donor (acceptor) concentrations we conclude that they belong to carbon-hydrogen-related defects consisting of one C and one H atom. The similar annealing behavior and identical depth profiles of E42 and E262 correlate them with two different charge states of the same defect. From a comparison with earlier calculations we attribute E42 to the double acceptor and E262 to the single acceptor state of the CH_{1AB} complex. In good agreement with the results of previous studies E90 is assigned to the acceptor state of the CH_{1BC} complex. Our preliminary Laplace

DLTS studies on SiGe with a Ge content <5% show different local Ge environments for E90 and H180 in the nearest and second-nearest neighborhood. We interpret this as an indication for a different origin of these defects. After annealing the samples under reverse bias at 320 K another CH-related defect (CH_B) can be detected by Laplace DLTS in *n*-type Si. Previously, this defect was often wrongly assigned to the single donor state of CH_{1BC}. The field dependence of the emission rate of CH_B identifies the level as a single donor state. However, the depth distribution of CH_B differs clearly from that of E90. Our results on the carbon-hydrogen complex give a conclusive explanation of previously reported controversial experimental data.

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1 Introduction Carbon and hydrogen are often present in Si crystals, and their interaction can lead to the formation of several electrically active CH-related complexes [1–5]. Five different configurations of the CH complex with one substitutional C and one H atom were previously predicted by theory [1]. A H atom located in the bond-centered position between C and a neighboring Si atom (CH_{1BC}) should be the most stable configuration in the negative and positive charge state of this defect. However, according to theory a H atom located between the two silicon atoms neighboring carbon (CH_{2BC}), a H atom directly bound to carbon in the anti-bonding position (CH_{1AB}), and a H atom located at the interstitial T_d position close to carbon (CH_{1Td}) were predicted to be only slightly less stable (around 0.1–0.2 eV) as compared to CH_{1BC}.

The activation enthalpies of the corresponding configurations that were obtained from *ab-initio* calculations [1] are combined in Table 1. One should notice that, according to theory, all of the CH configurations should introduce deep levels into the band gap of Si. However, until now no

indisputable experimental evidence of the presence of these defects in hydrogenated Si exists in the literature.

Previously, three dominant deep level transient spectroscopy (DLTS) peaks were often observed by conventional DLTS and high-resolution Laplace DLTS techniques after hydrogen introduction into silicon [1–5]. Two of them, with an activation enthalpy of E_C–0.16 eV (labeled differently in different studies CH_A [6], CH_I [1], or E90) and E_C–0.14 eV ((CH)_{II}) [1], appeared in the upper half of the Si band gap. The third level, labeled H180 [2], with an activation enthalpy of E_V+0.33 eV was often observed in the lower part of the band gap. CH_{II} [1] was observed only after implantation of hydrogen at low temperatures, and this defect is stable only below 225 K. In Ref. [1] the authors attributed this defect to the donor state of CH_{2BC}. The experimental results on the two other levels E90 and H180 are controversial. In some studies E90 was attributed to the single acceptor state of CH_{1BC} due to the absence of the enhancement of its emission rate with electric field [1, 6]. In contrast, in Ref. [3] an enhancement of the emission rate

of this defect as a function of electric field was observed, and therefore this level was linked with the donor state of $\text{CH}_{1\text{BC}}$. Similarly, some confusion about the origin of H180 exists in the literature. In Ref. [1] this level was attributed to the donor state of $\text{CH}_{1\text{BC}}$, whereas in Ref. [2] the same DLTS peak was tentatively assigned to the donor state of $\text{CH}_{1\text{AB}}$ due to a different annealing behavior of E90 and H180 under illumination.

Table 1 Calculated positions of the electrical levels of different configurations of the CH complex. All values are given in eV with respect to the conduction band.

Charge state	$\text{CH}_{1\text{BC}}$	$\text{CH}_{1\text{AB}}$	$\text{CH}_{1\text{Td}}$	$\text{CH}_{2\text{BC}}$	$\text{CH}_{2\text{AB}}$
(-0)	0.3	0.63	0.89		1.07
(0/+)	0.81	0.82	>1.12	0.4	

In the present study, we summarize our recent findings obtained by DLTS, Laplace DLTS and minority carrier transient spectroscopy (MCTS) techniques in hydrogenated *n*- and *p*-type Si with different concentrations of doping levels, C, O, and H, and in hydrogenated diluted SiGe alloys. We show that besides E90 and H180 two other CH-related defects (E42 (E262) and E90') can be often observed in samples subjected to hydrogenation by wet chemical etching or by a dc H plasma treatment. By analyzing DLTS and MCTS spectra together with Laplace DLTS data, obtained in diluted SiGe alloys with a low content of Ge, we demonstrate that H180 and E90 cannot belong to different charge states of the same defect, as suggested in Refs. [1, 3]. The origin of the CH-related traps is discussed. Our findings give a conclusive explanation of previously reported experimental and theoretical results.

2 Experimental procedure

Float-zone and Czochralski *n*- and *p*-type Si and SiGe wafers were studied. The doping level and concentrations of carbon and oxygen in these wafers are combined in Table 2. The wafers were cut into $10 \times 5 \text{ mm}^2$ samples and cleaned in acetone and di-ionized water. Hydrogen was introduced into the samples by wet chemical etching in CP4A ($\text{HF}:\text{HNO}_3:\text{CH}_3\text{COOH}$, 3:5:3) or from a remote dc hydrogen plasma at different sample temperatures. After the H treatment, the samples were dipped in HF, and Schottky contacts were fabricated by resistive evaporation of Au through a shadow mask onto the polished side of the sample. Ohmic contacts were made by rubbing eutectic InGa alloy onto the backside of the samples. The quality of the Schottky and Ohmic contacts was checked by current-voltage and capacitance-voltage (CV) measurements at room temperature and at 50 K. The CV curves were recorded at 1 MHz. Conventional DLTS, MCTS and high

resolution Laplace DLTS were used to investigate the electrical properties of deep level defects. The labeling of the DLTS and MCTS peaks in this work corresponds to the temperature at which the peaks were observed in the DLTS spectra for an emission rate of 50 s^{-1} . The depth profiles of the defects were calculated from the Laplace DLTS spectra by taking into account the λ -layer [7]. The electric field was calculated from the CV measurements as described in Ref. [7].

Table 2 Samples used in the present study: phosphorous (P) and boron (B) concentration as obtained from our CV measurements; substitutional carbon (C_s) and interstitial oxygen (O_i) concentration are given by the vendors.

Sample	Dopants	$[\text{N}_\text{d}] (\text{cm}^{-3})$	$[\text{C}_\text{s}] (\text{cm}^{-3})$	$[\text{O}_\text{i}] (\text{cm}^{-3})$
FZ1	P	1.5×10^{14}	5×10^{15}	$<1 \times 10^{16}$
FZ2	P	1×10^{14}	5×10^{15}	$<1 \times 10^{16}$
FZ3	P	1×10^{15}	5×10^{15}	$<1 \times 10^{16}$
FZ4	P	5×10^{15}	5×10^{15}	$<1 \times 10^{16}$
CZ1	B	1×10^{15}	6×10^{17}	1×10^{18}
CZ2	P	1×10^{15}	5×10^{15}	1×10^{18}
CZ3	P	2×10^{15}	8×10^{16}	3×10^{17}
SiGe1	B	2.5×10^{14}	5×10^{15}	unknown
SiGe2	P	3.5×10^{15}	5×10^{15}	unknown

3 Experimental results Figure 1 shows conventional DLTS and MCTS spectra recorded in *n*-type FZ-silicon samples subjected to hydrogenation by wet chemical etching (Fig. 1a) or by a H plasma treatment at 373 K (Fig. 1b).

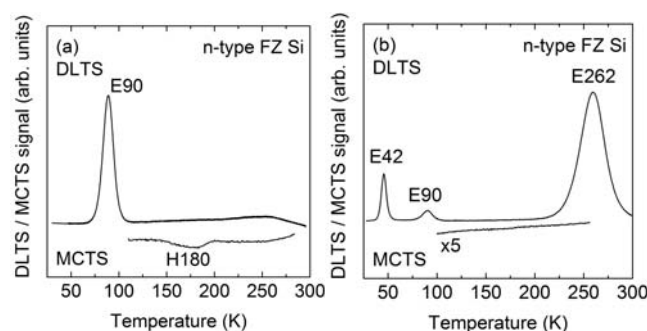


Figure 1 Conventional DLTS and MCTS spectra recorded in *n*-type FZ silicon samples (FZ1) subjected to hydrogenation by wet chemical etching (a) or by a H plasma treatment at 373 K (b). The spectra were recorded with the following parameters: $e_n = 50 \text{ s}^{-1}$, $V_\text{R} = -2 \text{ V}$, $V_\text{P} = 0 \text{ V}$, and $t_\text{p} = 1 \text{ ms}$.

Figure 2 shows a conventional DLTS spectrum recorded in *p*-type FZ silicon subjected to hydrogenation by a dc H plasma treatment at 373 K. Similar spectra are also observed after wet chemical etching and at lower temperatures of the H plasma treatment, varying in the range of 313–373 K. All DLTS peaks observed in Figs. 1 and 2 consist of only one Laplace DLTS peak (not shown). After wet chemical etching only one dominant peak, labeled E90, is observed in the DLTS spectrum, and one peak H180 is detected in the MCTS spectrum. Besides E90, two other DLTS peaks E42 and E262 are detected in samples subjected to hydrogenation by a dc H plasma treatment. However, no MCTS peaks are observed in the range of 100–300 K.

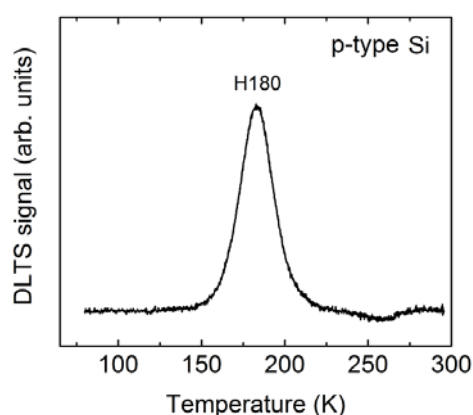


Figure 2 Conventional DLTS spectrum recorded in *p*-type CZ silicon (CZ1) subjected to hydrogenation by a dc H plasma treatment at 373 K. The spectrum was recorded with the following parameters: $e_n = 50 \text{ s}^{-1}$, $V_R = -2 \text{ V}$, $V_p = -0 \text{ V}$, and $t_p = 1 \text{ ms}$.

The electrical properties of E42, E90, and E262, as obtained from the Laplace DLTS measurements, are presented in Refs. [6, 8]. The activation enthalpy of H180 is 330 meV and its apparent capture cross section is $5 \times 10^{-16} \text{ cm}^2$. Direct measurements of the capture cross section of E42, E90, and E262 at different temperatures show no barrier for electron capture. However, similar measurements for H180 give a barrier for the capture of holes of around 53 meV. The entropy change following the emission process is 1.6 k and the capture cross section obtained by extrapolating to $T = \infty$ is $1 \times 10^{-16} \text{ cm}^2$.

E42 and E90 exhibit a slight enhancement of their emission rate with the electric field, as presented in Refs. [6, 8]. This enhancement is significantly smaller than that expected in the frame of the Poole-Frenkel model [9] for a defect with a Coulombic attractive potential. In Refs. [6, 8] we show that the enhancement of the emission rate of E42 can be well described by a Morse potential, whereas that of E90 by a model with a square well potential. No enhancement of the emission rate of E262 was observed [8]. Therefore, we correlate E42 with a double acceptor, and E90 and E262 with a single acceptor. No enhancement of the emission rate of H180 is observed in the range of 2500–22500

V/cm. This result is consistent with the findings reported previously in Ref. [2].

As mentioned in the introduction, E90 and H180 were correlated with CH-related defects with one C and one H atom. However, until now the assignment of H180 to a CH-related defect with one hydrogen atom is very speculative. In order to confirm this hypothesis we used the approach developed in Ref. [10]. Feklisova and Yarykin [10] showed that the slope of the reduction of the concentration of a H-related complex towards the bulk is proportional to the number of hydrogen atoms in this complex. However, the number of H atoms cannot be directly determined by measuring the depth profile. The comparison with the depth profile of another defect that contains a known number of H atoms is necessary in order to draw conclusions about the number of H atoms in the complex under investigation. We determine the depth profile of H180 after wet chemical etching (Fig. 3) and compare it with that of the boron-hydrogen (BH) complex in the sample. The concentration of the BH complex is obtained by subtraction of the concentration of shallow acceptors (B) in the hydrogenated samples from their initial concentration before hydrogenation. The depth profiles of BH and H180 are decreasing towards the bulk of the sample and the concentration of BH is significantly higher than that of H180. However, the slope of the reduction of the concentration is identical and therefore, according to Ref. [10], we conclude that H180 and BH contain an equal number of H atoms.

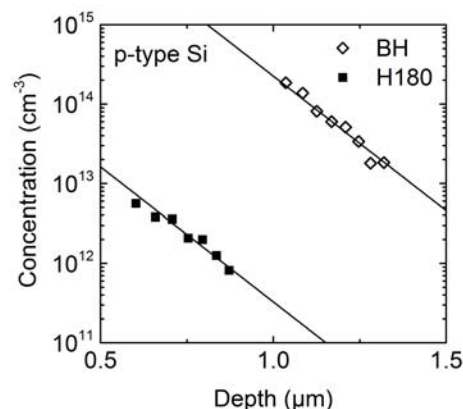


Figure 3 Concentration depth profiles of H180 recorded in *p*-type CZ-Si (CZ1) after wet etching in CP4A. The solid line is a guide to the eye and it shows the identical reduction of the defect concentration.

The isochronal annealing of the defects shows that E42 and E262 anneal out identically (Fig. 4a). Moreover, these peaks appear always together in different samples with different doping levels, C, O, and H concentrations. Therefore, we correlate these peaks with different charge states of the same defect. A comparison of the depth profiles of E42 (E262) and E90 shows that the slope of the reduction of the concentration is identical and therefore both defects contain the same number of hydrogen atoms (see Ref. [8]). An

increase in the concentration of C also increases the concentration of E262 (E42) (Fig. 4b), whereas the concentration of this defect remains constant when the doping concentration or the oxygen concentration is varied. Therefore, it seems that E262 (E42) is also a CH-related complex with one C and one H atom.

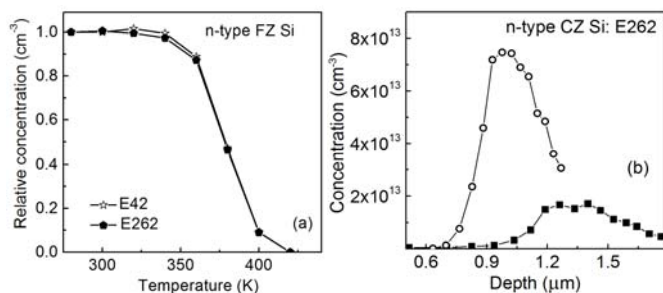


Figure 4 (a) Relative concentrations of E42 and E262 recorded in the FZ2 sample after 60 min. isochronal annealing steps at different temperatures. (b) The depth profile of E262 recorded in CZ2 and CZ3 samples with different C concentration.

One should also notice that the reverse bias annealing (RBA) of hydrogenated samples leads to the appearance of an additional peak E90', which can be resolved only by the Laplace DLTS technique. Figure 5 shows different Laplace DLTS spectra recorded in samples with different doping concentrations. The RBA steps are performed with the reverse bias of -4 V at 320 K in all samples. Only one Laplace DLTS peak E90 is observed in the sample with a doping concentration of $1 \times 10^{14} \text{ cm}^{-3}$. In contrast, two peaks E90 and E90' are detected in samples with higher doping levels. By a careful analysis of the depth profiles we showed that E90' was another CH-related complex [6]. E90' is a single donor, and the enhancement of its emission rate fits perfectly to the Poole-Frenkel model.

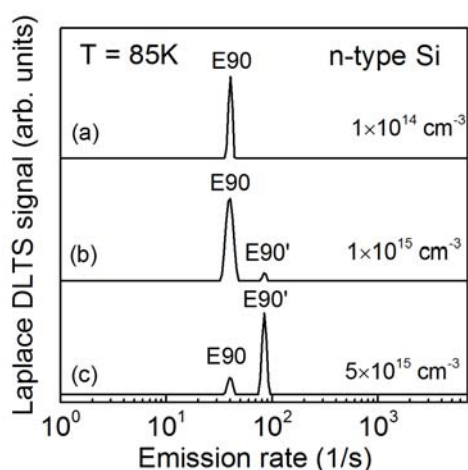


Figure 5 Laplace DLTS spectra recorded after a reverse bias annealing with -4 V at 320 K in samples with different doping levels (FZ2 (a), FZ3 (b), and FZ4 (c)).

The analysis of Laplace DLTS spectra in diluted SiGe alloys can also bring additional information about the structure of defects. Generally, a point defect in Si appears as a single Laplace DLTS peak at a definite temperature (see Fig. 5a). In contrast, an alloy splitting effect, which leads to appearance of a number of Laplace DLTS peaks (dominant peaks and their satellites) can be often observed in diluted SiGe alloys [11–13]. The appearance of the dominant peaks and their satellites in SiGe was previously interpreted by the presence of a different number of Ge atoms in the nearest and second-nearest neighborhood of the defect [11–13]. Moreover, for different defects the relative intensities of the dominant peaks and their satellites can vary depending on the structure of defects. Thus, a significant overpopulation of B close to Fe and a neighboring Ge atom comparing with that expected from theory was reported in Ref. [12, 13] whereas isolated Fe was randomly in SiGe alloys distributed without any preferential location. Similarly, the comparison of Laplace DLTS spectra of E90 and H180 in SiGe alloys should give similar results with equal concentration ratios between dominant peaks and their satellites if the peaks belong to different charge states of the same defect.

Figure 6 shows Laplace DLTS spectra recorded in *n*- and *p*-type SiGe samples subjected to hydrogenation by a dc H plasma treatment at 313 K or 373 K. The Ge content is approximately 4.5 % in all samples. We emphasize that the Laplace DLTS spectra recorded at similar temperatures in pure Si show single delta peaks, which can be correlated with E42, E90, E262, and H180 (see Figs. 1 and 2). In contrast, the Laplace DLTS spectra recorded in samples with a small Ge content differ significantly from those obtained in pure Si. In these spectra a number of dominant Laplace DLTS peaks together with their satellites are detected in both *n*- and *p*-type SiGe.

The Laplace DLTS spectra recorded at 47 K and 265 K in *n*-type SiGe and at 170 K in *p*-type SiGe have some similarities: they consist of one dominant peak, labeled E42_{SiGe} (47 K), E262_{SiGe} (265 K), and H180_{SiGe} (170 K), respectively, and a number of left-handed (170 K) or right-handed (47 K and 265 K) satellites. The relative intensity of these satellites increases with the Ge content in the sample. Therefore, similar to the findings of Refs. [11–13], we assign the dominant peaks to defects also observed in pure Si with no Ge atoms in their nearest neighborhood. The small satellites are interpreted as the same defect but with a different number of Ge atoms in the nearest and the second-nearest shell. The left-handed satellites in *p*-type SiGe and right-handed satellites in *n*-type SiGe can be explained by the same Ge composition in the neighboring shells. Ge in the neighborhood of CH leads to a shift of the electrical levels towards the conduction band edge. H180_{SiGe} is broad and we are not able to resolve its fine structure (second-nearest neighborhood). This is mainly due to the poorer resolution of the Laplace DLTS technique at higher temperatures and a significantly smaller intensity of the

H180_{SiGe} signal as compared to those observed in *n*-type samples. Dobaczewski et al. [14] showed that the resolution of the Laplace DLTS technique depended on the signal-to-noise ratio, which was significantly worse for our *p*-type samples in comparison to the *n*-type samples.

The Laplace DLTS spectra recorded at 85 K in *n*-type SiGe differ considerably from those analyzed above. Two dominant peaks E90_{SiGe} and E80_{SiGe} are observed and their intensities are comparable. The relative intensity of E80_{SiGe} to E90_{SiGe} increases with the Ge content in the samples. Therefore, one can conclude that E90_{SiGe} originates from the same defect as E90 in pure Si, whereas E80_{SiGe} is a defect similar to E90 but with one additional Ge atom in its nearest neighborhood. One should also notice that already at 4.5 % of Ge the intensity of E80_{SiGe} is comparable to that of E90_{SiGe}. Under the assumption of a random distribution of Ge in Si (see, for example, the relative intensities between the dominant peaks and their satellites for E42, E262, and H180) a significantly lower intensity of this peak is expected. This observation indicates that hydrogen prefers to be located between the C atom and a neighboring Ge atom. Besides these dominant peaks we also observed a number of satellites. Their intensity also depends on the Ge content of the samples, and the defects corresponding to these peaks contain a different number of Ge in their second-nearest shell. A detailed analysis of these peaks will be presented in Ref. [15].

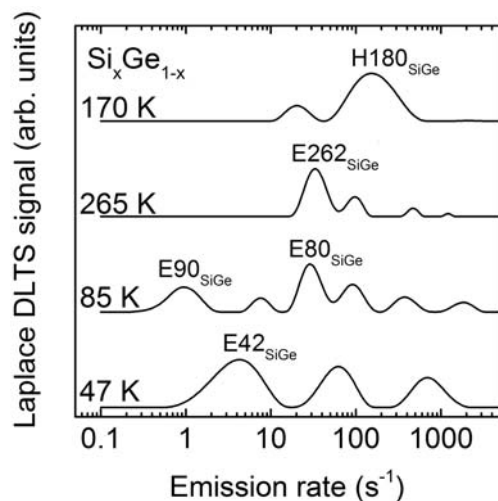


Figure 6 Laplace DLTS spectra recorded in *n*- and *p*-type Si_{1-x}Ge_x samples (SiGe1 and SiGe2) subjected to hydrogenation by a dc H plasma treatment at 313 K or 373 K. The Ge content was approximately 4.5 % in all samples.

4 Discussion Our study shows that the different experimental results obtained in *n*-type Si in Refs. [1, 3, 16] can be explained by different preparation procedures of the samples used in these studies. For an increase of the intensity of E90 a reverse bias annealing (RBA) was always used in Ref. [3], whereas no annealing was performed after

implantation of protons in Ref. [1]. We demonstrate that RBA results in the formation of another CH-related defect (E90' or CH_B) which has similar electrical properties (activation enthalpy and apparent capture cross section) as E90. Both these defects can be only resolved by the high-resolution Laplace DLTS technique. The careful comparison of the emission rates of E90 and E90' as a function of electric field shows that these defects also have different charge states: the single donor state (E90') and the single acceptor state (E90). The presence of different defects before and after RBA explains the inconsistency observed previously in Refs. [1, 3, 16].

E42 and E262 have identical annealing behaviors and their depth profiles are also found to be always identical in different FZ and CZ Si samples hydrogenated by wet chemical etching or by a dc H plasma treatment. Therefore, we assign these peaks to the double acceptor state (E42) and to the single acceptor state (E262) of the same defect. By comparison with theory [1] this defect can be attributed to CH_{1AB}. The detailed analysis of E42 and E262 is presented in Ref. [8].

The results shown above suggest that E90 and H180 cannot belong to different charge states of the same defect. Indeed, we do not observe H180 in the MCTS spectrum (Fig. 1b) recorded in samples subjected to a dc H plasma treatment, although E90 appears in the DLTS spectrum recorded in the same sample. Also, the Laplace DLTS spectra obtained in *n*-type and *p*-type SiGe samples with a Ge content of 4.5 % are very different. The spectrum recorded at 170 K in *p*-type SiGe consists of one dominant peak and a left-handed satellite whereas two Laplace DLTS peaks with similar intensities and a number of satellites were observed at 90 K in *n*-type SiGe samples. During the hydrogen introduction at 373 K the Fermi level lies below E90 and above H180. According to theory, most of the hydrogen is expected to be positively charged at this temperature in SiGe with a low Ge content [17]. Then, if these peaks belong to different charge states of the same defect one would expect a similar pattern of the Laplace DLTS peaks of E90 and H180. A preference of H to be located between a C atom and a neighboring Ge atom is detected only for E90, whereas this effect is not observed for H180.

We also rule out that H180 originates from the same defect as E42 (E262). Again H180 is not observed in the MCTS spectrum in Fig. 1b, although both E42 and E262 are detected in the DLTS spectrum of the sample. Therefore, it seems reasonable to suggest that E90, E42 (E262), and H180 belong to different configurations of the CH complex.

H180 was previously assigned to a donor state of a CH-related defect [2]. For a single donor in *p*-type Si its potential can be approximated by a square-well potential. In this case a slight enhancement of the emission rate of H180 is expected [9]. Similarly, in Ref. [18] the authors suggested that a Morse potential could approximate the repulsive Coulombic interaction which is characteristic for a

double donor. In this case also a slight enhancement of the emission rate should be observed (compare Fig. 3). However, we do not observe any changes of the emission rate of H180 for electric fields varying in the range of 2500–23000 V/cm.

Similar to the EL2 defect in GaAs described in Ref. [18], the absence of an enhancement of the emission rate of H180 can be correlated with the capture barrier of 53 meV. Under these conditions H180 can be assigned to a single acceptor.

Theory predicts five different configurations of the CH-complex in hydrogenated Si. The thermally unstable $\text{CH}_{2\text{BC}}$ was identified by Andersen *et al.* by combining uniaxial stress measurements together with the Laplace DLTS technique [1]. Two other configurations of the CH complex (E42 (E262) and E90) with one C and one H atom were observed in our previous studies. The results presented above show unambiguously that H180 is also a CH-complex with one H atom and its configuration is different from E42 (E262), $\text{CH}_{2\text{BC}}$, and E90 ($\text{CH}_{1\text{BC}}$).

The calculated level position of the $\text{CH}_{1\text{Td}}$ acceptor state [1] agrees reasonably well with that of H180 observed in the present study. The absence of a field effect, that would be expected for an acceptor state, can be explained by the presence of a capture barrier. Therefore, we tentatively assign H180 to the single acceptor state of $\text{CH}_{1\text{Td}}$. A schematic sketch of the detected CH level positions is presented in Fig. 7.

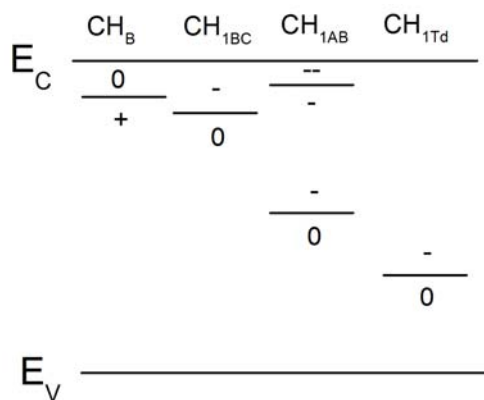


Figure 7 Schematic level position of different configurations of the CH complex in hydrogenated *n*- and *p*-type Si.

5 Conclusions Several deep level traps E42, E90, E262, and H180 were observed in *n*-type and *p*-type Si subjected to hydrogenation by wet chemical etching or a dc H plasma treatment. We showed that E42 and E262 belonged to different charge states of the same CH-related defect with one H atom and one C-atom. By comparing our findings with theory we attributed E42 to the double acceptor and E262 to the single acceptor state of the $\text{CH}_{1\text{AB}}$ complex and E90 was assigned to the acceptor state of the $\text{CH}_{1\text{BC}}$ complex. From the analysis of the depth profile of

H180 we showed that this defect contained only one H atom. We did not observe an enhancement of the emission rate of this defect but it exhibited a barrier for capture of holes of around 53 meV. The comparison of the MCTS and DLTS spectra in *n*-type and *p*-type Si and a different pattern of the Laplace DLTS spectra of E90 and H180 recorded in SiGe with a low Ge content showed that E42 (E262), E90 and H180 belonged to different configurations of the CH complex. By a comparison with theory we tentatively identified H180 with the $\text{CH}_{1\text{Td}}$ configuration.

After reverse bias annealing we detected another CH-related defect E90', with a similar activation enthalpy and apparent capture cross section as E90. This defect introduced a single donor level into the band gap of Si and it was concluded to be CH-related defect different to E90. In the present study we gave a conclusive explanation of previously reported controversial experimental data on the carbon-hydrogen complex.

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