

# Carbon-hydrogen-related complexes in Si

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## ABSTRACT

Several deep level transient spectroscopy (DLTS) peaks (E42, E65, E75, E90, E262, and H180) are observed in *n*- and *p*-type Czochralski-grown Si samples subjected to hydrogenation by a dc H plasma treatment. The concentration of the defects is found to be proportional to the carbon and hydrogen content in our samples. The analysis of the depth profiles performed in Si samples hydrogenated by wet chemically etching shows that all these defects contain a single H atom. E65 and E75 appear only in samples with a high oxygen content which shows that oxygen is a constituent of these defects. The analysis of the enhancement of the emission rate of the defects with electric field shows that E65, E75, E90, and E262 are single acceptors whereas E42 is a double acceptor. The presence of a barrier for hole capture (about 53 meV) can explain the absence of the enhancement of the emission rate of H180, which can be attributed to a single acceptor state. From a comparison with theory, we assign E90 to CH<sub>1BC</sub>, E42 (E262) to CH<sub>1AB</sub>, and H180 to CH<sub>1Td</sub>. The similarity of the electrical properties of E65 and E75 to those of E90 suggest that E65 and E75 may originate from the CH<sub>1BC</sub> defect with an oxygen atom in its nearest neighborhood. Our results on the CH-related complexes give a conclusive explanation of some previously reported controversial experimental data.

## 1. Introduction

The performance of electronic devices can be greatly influenced by the presence of unintentionally introduced electrically active defects in silicon. Some impurities such as carbon or oxygen, which are electrically inactive in Si, can create electrically active complexes by interaction with other crystal imperfections and impurities. Nowadays the technological processing of devices often includes heat treatments of Si wafers in hydrogen (H) containing atmosphere in order to reduce the density of interface states or to passivate the electrical activity of the surface. As a result, hydrogen penetrates into the bulk of Si wafers where it leads to the appearance of a number of H-related defects in the active region of devices. Among those traps the electrical and structural properties of CH-related defects attract significant attention, since carbon is always present in both Czochralski (Cz) and float-zone (FZ) Si. Until now the experimental results concerning the CH-related defects are controversial. Generally, two CH-related deep level transient spectroscopy DLTS peaks, labeled E(0.16) and H1 in Refs. [1,2], can be observed in hydrogenated *n*-type and *p*-type Si with a low oxygen content [1,2]. E(0.16) and H1 were shown to be C- and H-related defects [1,2]. However, the charge state and exact origin of these defects are still under discussion [1–4]. Theory predicts the appearance of different

configurations of CH-related defects in Si [3]. We emphasize that Yoneta et al. [5] reported that in *n*-type Si samples with a high O content (around 10<sup>18</sup> cm<sup>-3</sup>) E3 (E(0.16) in Ref. [1]) was not dominant in the DLTS spectrum. Besides E3 some other peaks labeled E1 and E2 appeared in hydrogenated *n*-type Si samples with a high O content. In Ref. [5] the authors suggested that these peaks could be correlated with COH-related defects since their concentration increased with the O and C content. However, the exact nature of these defects is still unknown. Some DLTS peaks were also recently reported in the lower part of the bandgap of Cz Si with a high oxygen content of about 13–17.5 ppma [6]. The authors attributed these peaks to the O<sub>2</sub>-H defect. In the present study we review our recent findings [4,7–9], which shed light on the origin of carbon-hydrogen related complexes in *n*-type and *p*-type Si samples with different oxygen concentrations. Our results on the CH-related complexes give a first conclusive explanation of some previously reported controversial experimental data.

## 2. Experimental procedure

Samples were cut from different *n*-type and *p*-type Czochralski (Cz) and Float-Zone (FZ) Si wafers with a doping level of about

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$2 \times 10^{15} \text{ cm}^{-3}$  and different concentrations of carbon and oxygen. Hydrogen was introduced by wet chemical etching at room temperature for 2 min in an acid consisting of  $\text{HNO}_3:\text{HF}:\text{CH}_3\text{COOH}$  with a volume ratio of 5:3:3 or by a dc H plasma treatment performed at 320 K or 370 K. Schottky diodes were produced by resistive evaporation of Au (*n*-type Si) or Al (*p*-type Si) in vacuum onto the polished side of the samples at room temperature. Ohmic contacts were prepared by rubbing the backside of the samples with an eutectic InGa alloy. The quality of the Schottky and Ohmic contacts was characterized by current-voltage (*I*-*V*) measurements in the range of 50–300 K. Capacitance-voltage (*C*-*V*) measurements were performed at 1 MHz. Laplace DLTS [10] with two filling pulses was employed to investigate the electronic properties (activation enthalpy, capture cross section, charge state) of deep levels and their depth profiles. The labeling of the DLTS peaks in this work corresponds to the temperatures at which the peaks were observed in the DLTS spectra for an emission rate of  $48 \text{ s}^{-1}$ . Deep level concentration profiles were measured at a fixed reverse bias while varying the two pulse biases. The electrical field was calculated from the *C*-*V* profile as described in Ref. [11]. The field effect has been investigated at fixed pulse biases while varying the reverse bias.

### 3. Results

Fig. 1 shows DLTS spectra recorded in *n*-type Cz Si ( $[\text{O}_i] \sim 1 \times 10^{18} \text{ cm}^{-3}$ ,  $[\text{C}_s] = 5 \times 10^{15} \text{ cm}^{-3}$ ) after hydrogenation by a dc H plasma treatment. Several DLTS peaks (E42, E65, E75, E90, E120, and E262) were observed after hydrogenation. In contrast, no DLTS peaks were detected in this sample before hydrogenation. One should also emphasize that all these defects except E120 were observed in Si samples after wet chemical etching [4,7–9] and, therefore, we rule out that they were generated by the damage of the crystal lattice during the dc H plasma treatment. In order to investigate the electrical and annealing properties of E42, E65, E75, E90, and E262 the high-resolution Laplace DLTS technique was employed. All DLTS peaks consisted of single Laplace DLTS lines and no fine structure was observed. Information about the charge state of a defect can be obtained from the analysis of the shift of the emission rate of a defect under different reverse biases [12]. The emission rates of E42, E65, E75, E90, and E262 were indeed enhanced with the electric field. However, this enhancement was significantly weaker compared to that expected from the three-dimensional Poole-Frenkel model [12]. A model of a square-well potential, which is characteristic for neutral defects, describes well the enhancement of the emission rates of E65,

**Table 1**

The electrical properties of the defects observed in Figs. 1 and 3. Their assignment from this study is also presented.

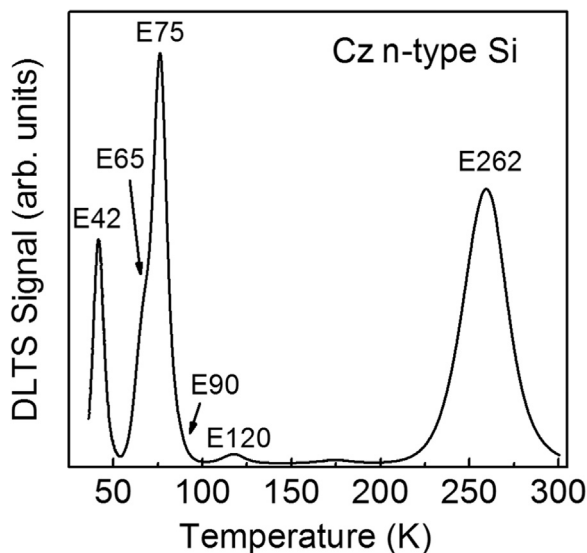
Defect	Activation enthalpy (meV)	Apparent capture cross section ( $\text{cm}^{-2}$ )	Charge state	Assignment
E42	60	$2 \times 10^{-17}$	(-/-)	$\text{CH}_{1\text{AB}}$
E65	110	$1.4 \times 10^{-16}$	(-/0)	$\text{CH}_{1\text{BC}} + \text{O}_i$
E75	130	$8.6 \times 10^{-16}$	(-/0)	$\text{CH}_{1\text{BC}} + \text{O}_i$
E90	160	$2.2 \times 10^{-16}$	(-/0)	$\text{CH}_{1\text{BC}}$
E90'	140	$2.8 \times 10^{-16}$	(0/+)	$\text{CH}_n (n > 1)$
E262	510	$2 \times 10^{-15}$	(-/0)	$\text{CH}_{1\text{AB}}$
H180	330	$5 \times 10^{-16}$ (barrier 53 meV)	(-/0)	$\text{CH}_{1\text{Td}}$

E75, E90, and E262 [12]. Details on these experimental results are given in Refs. [4] (E90), [7] (E65, E75), and [8] (E262). Based on these experimental findings we conclude that these defects are single acceptors in *n*-type Si. In contrast, the enhancement of E42 is characteristic for a double-acceptor in *n*-type Si and it is modelled by an inverted Morse potential [8,13]. The assignment of E65, E75, E90, and E262 to single acceptors and E42 to the double acceptor state is also consistent with the order of magnitude of the apparent capture cross section of the defects (see Table 1) since the capture cross section of E42 is significantly smaller compared to other defects from Fig. 1.

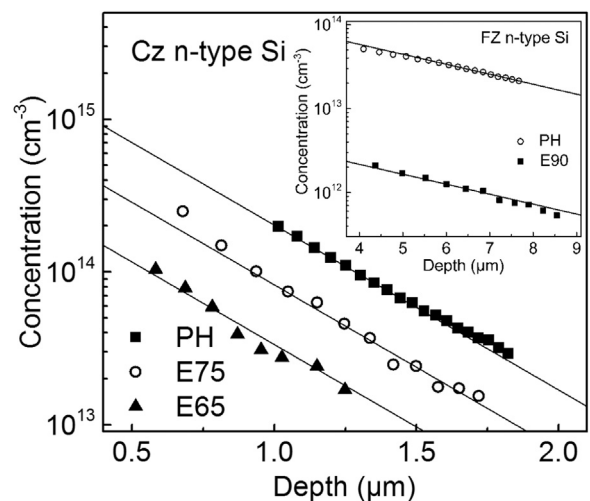
As mentioned in the introduction, E65, E75, and E90 have been already observed in previous studies [4,5]. There was shown that they contained carbon and hydrogen (E65, E75, E90), as well as oxygen (E65, E75). However, the number of H atoms in E65 and E75 is still unknown.

In order to shed light on the nature of these defects we employed the approach that was suggested in Ref. [14]. In this study, Feklisova and Yarykin demonstrated that after wet chemical etching (WCE) the reduction of the concentration of H-related defects with depth should be identical if they contained identical numbers of H atoms. One should emphasize that this method is also valid even if the concentration of the H-related defects is not the same.

Following this idea, depth profiles of E65 and E75 recorded after WCE for 5 min at room temperature are compared in Fig. 2. The concentration depth profile of the phosphorous-hydrogen (PH) complex is also presented in this figure. The PH concentration was calculated by subtracting the concentration of the net free carrier concentration in as-grown samples from the concentration observed after WCE. The introduction of H lead to the passivation of phosphor-



**Fig. 1.** DLTS spectrum recorded in *n*-type Cz Si subjected to hydrogenation by a dc H-plasma treatment.



**Fig. 2.** The depth profiles of E65, PH, and E75 recorded in a Cz Si sample after WCE for 5 min at room temperature. The solid lines shows an identical slope for the concentration of the defects. The inset shows the depth profiles of E90 and PH in a FZ Si sample after WCE at room temperature.

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