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D. Cavalcoli, A. Cavallini, E. Gombia. Energy Levels Associated with Extended Defects in Plastically Deformed n-Type Silicon. *Journal de Physique III*, 1997, 7 (7), pp.1399-1409. 10.1051/jp3:1997195 . jpa-00249653

**HAL Id: jpa-00249653**

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Submitted on 4 Feb 2008

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# Energy Levels Associated with Extended Defects in Plastically Deformed n-Type Silicon

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*(Received 3 October 1996, revised 9 January 1997, accepted 27 January 1997)*

PACS 61.72.Ff – Direct observation of dislocations and other defects

PACS 61.72.Lk – Linear defects: dislocations, disclinations

PACS.71.20.Mq – Elemental semiconductors

**Abstract.** — Deep Level Transient Spectroscopy (DLTS) investigations of plastically deformed, n-type silicon have been performed. DLTS spectra revealed four lines usually found in deformed silicon but they were unusually dominated by a broadened level located at 0.40 eV from the conduction band edge. This trap resulted to be the most localized at the dislocations, while the other traps are probably related to point defects. The measured DLTS line widths have been simulated by the introduction of a broadening parameter  $\delta$ , whose dependence on the dislocation density has been studied. Some hypotheses on the physical mechanisms responsible for the line broadening have been advanced. A tentative identification of the defects responsible for the deep levels observed has been performed.

## 1. Introduction

The electronic properties of extended defects have been studied for many years by several groups [1–5]. Nevertheless the question which energy levels in the band gap are due to dislocations is far to be understood as plastic deformation introduces, besides dislocations, a large amount of point defects in the crystal. Since the investigated electrical properties are mainly due to point defect effects, it is often difficult to separate the point defect from the extended defect contributions. Moreover Deep Level Transient Spectroscopy (DLTS) needs careful analysis when applied to Plastically Deformed (PD) silicon since severe problems must be taken into account: i) the band bending induced by electronic charges confined at dislocations induces a change of the capture and emission properties of the electronic levels during filling and emptying of the traps, ii) the “logarithmic filling time behaviour” often occurs [1], iii) the capacitance transients are often non exponential [1], which gives broadened DLTS peaks. Notwithstanding these difficulties a comparison of the wide literature results leads to the identification of four traps labelled A, B, C and D [1], whose corresponding DLTS peaks are strongly dependent on the deformation and annealing procedures.

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Table I. — *Details of the deformation procedure.  $T_d$  is the deformation temperature,  $\tau$  the resolved shear stress,  $\tau_i$  the dislocation incubation time.*

Sample	$T_d$ (°C)	$\tau$ (MPa)	duration (h)	$\tau_i$ (s)
DAT1	650	38	60	$1.8 \times 10^5$
DAT3	750	25	24	$7.0 \times 10^3$

In this paper DLTS analyses of PD n-type Si will be reported. The starting material, lightly doped, underwent a weak deformation that introduced a relatively low dislocation density  $N_D$ . DLTS spectra showed in some cases unbroadened peaks that could be clearly resolved, in other cases broadened and overlapping peaks. The physical mechanisms contributing to line broadening have been analyzed. The capture mechanism of the most related to dislocations among the DLTS lines has been studied and some hypotheses on the identity of the deformation induced traps have been advanced.

## 2. Experimental and Methods

High purity, float-zone, n-type, {111} Si single crystals, grown by Wacker Chemitronic, were used in this study. The doping level  $N_d$  was equal to  $5 \times 10^{13}$  (phosphorus atoms)  $\text{cm}^{-3}$ . Sample bars of  $(5 \times 20)$   $\text{mm}^2$ , with the longest edge along the [110] axis, were plastically deformed by creep (four-point bending) along the [112] direction in a reducing atmosphere of forming gas (92% $\text{N}_2$ , 8% $\text{H}_2$ ) in a quartz and nuclear graphite deformation apparatus. The plastic strain ranges from 1 to 1.5%. Further details are reported in Table I. The load has been removed after deformation before cooling the sample to room temperature (the cooling rate was about  $4^\circ\text{C min}^{-1}$ ), therefore a partial annealing must be taken into account especially for the samples deformed at the highest temperature, so that a relaxation of the defect structure could possibly occur. In the DAT1 samples the dislocation density ranges from  $10^3$  to  $10^7$   $\text{cm}^{-2}$ , while in DAT3 from  $10^3$  to  $10^8$   $\text{cm}^{-2}$ . From each deformed bar, a set of samples has been obtained: each of them,  $(5 \times 2)$   $\text{mm}^2$  wide and with the longest side along the [112] direction, has a nearly uniform dislocation density. All the samples have been investigated by DLTS. Schottky diodes have been obtained by Au evaporation, while the ohmic contact by rubbering a Ga-In amalgam on the back surface. Both contacts have been formed at room temperature. The diodes have been tested by  $I$ - $V$  (Current-Voltage) plots to evaluate the series resistance, and by  $C$ - $V$  (Capacitance-Voltage) to determine the effective free carrier concentration. Hall effect and thermoelectric power measurements have been performed in order to check for compensation effects. DLTS measurements were performed by lock-in type spectrometer of high sensitivity. Details of the experimental apparatus can be found in reference [6].

In many cases the observed transients are, for non trivial reasons, non exponential giving rise to a broadening in the DLTS peaks [7]. In these cases the actual value of the activation energy  $E_a$  ( $E_a = \Delta H = \Delta G + T\Delta S$ , with  $\Delta H$  change in enthalpy,  $\Delta G$  change in Gibbs free energy and  $\Delta S$  change in entropy due to the ionization of the trap) is often questioned. The thermal emission rate  $e_n$  is given by:

$$e_n = \sigma_n v_{th} N_{CB} \times \exp\left(-\frac{\Delta G}{kT}\right) = \sigma_n v_{th} N_{CB} X_n \times \exp\left(-\frac{\Delta H}{kT}\right) = A_{pf} \times \exp\left(-\frac{\Delta H}{kT}\right) \quad (1)$$

where  $A_{pf} = N_{CB}(v_{th})\sigma_n X_n$  with  $X_n = \exp\left(\frac{\Delta S}{k}\right)$ ,  $\sigma_n$  capture cross-section and  $v_{th}$  thermal

velocity. To describe broadened DLTS peaks, the authors of reference [7] introduced a Gaussian distribution of ionization enthalpies so that the transient becomes:

$$C(t) = C(0) \int_{-\infty}^{\infty} G(E) \times \exp[-e_n(E)t] dE$$

where  $G(E)$  is a Gauss curve centred around  $E_a$  and normalized so that the area below the curve is unity:  $G(E) = \frac{1}{\delta\sqrt{2\pi}} \exp\left[-\frac{(E - E_a)^2}{2\delta^2}\right]$  with  $\delta$  the standard deviation of the Gaussian enthalpy distribution. The parameters of each DLTS line to be fitted with this model are: the prefactor  $A_{\text{pf}}$ , the activation enthalpy  $E_a$  the FPHW (full peak half width) of the Gaussian enthalpy distribution:  $\text{FPHW} = \delta\sqrt{2 \ln 2}$ , and the amplitude  $C(0)$  of the transient. For an ideal point defect, the capture cross-section is deduced from the change in the DLTS signal amplitude  $\Delta C$  as a function of the filling time  $t_p$ , according to [1]:

$$\Delta C(t_p) = \Delta C_{\text{max}}[1 - \exp(-n\langle v_{\text{th}} \rangle \sigma_n t_p)] \quad (2)$$

with  $n$  majority carrier concentration, *i.e.* from a plot of  $\ln(\Delta C)$  *vs.*  $t_p$  one can calculate  $\sigma_n$  if  $n$  and  $\langle v_{\text{th}} \rangle$  are known. For defects in plastically deformed materials, experimental results show that the capture kinetics is more complicated *i.e.* described by a logarithmic law: a model has been proposed [3] which describes the capture kinetic by a time dependent potential barrier  $\phi(t)$  built up by the carriers captured at the dislocations. The rate equation for the electron capture can be described by:  $\frac{dn_{\text{T}}}{dt} = (N_{\text{T}} - n_{\text{T}})n\langle v_{\text{th}} \rangle \sigma_n \exp\left[-\frac{q\phi(t_p)}{kT}\right]$  where  $n_{\text{T}}$  represents the number of electrons captured by the defects of density  $N_{\text{T}}$ . In the present work this model has been adopted due to the observed logarithmic filling time behaviour. The trap densities have been obtained by DLTS spectra measured with filling pulses longer than 100  $\mu\text{s}$  where all the DLTS peaks reach the saturation value.

### 3. Results

The following activation enthalpy values  $\Delta H$  (eV) have been found by the DLTS investigations in all the deformed samples:  $E(0.19)$ ,  $E(0.29)$ ,  $E(0.40)$  and  $E(0.56)$ , where the symbol  $E$  means that the energy values have been counted from the edge of the conduction band. Since these energy levels have been previously found in plastically deformed silicon [1] and labelled A, B, C and D respectively, the same notation as in reference [1] will be used from now on. In Figure 1 a comparison between DLTS spectra referring to the most deformed samples of DAT1 and DAT3 sets are reported. The C peaks are broadened and asymmetric, as sometimes occurs in dislocated samples. In particular in DAT3 samples the broadened C peak hides the D one, which is instead observed in the less deformed samples (Fig. 3), while in DAT1, the C level consists of two peaks, labelled  $C_1$  and  $C_2$ . In Figure 2 the thermal emission rates  $e_n$  ( $T^2$  corrected) relative to the A and C levels are reported as a function of  $1/T$  for samples deformed at different deformation temperatures  $T_d$ . The main difference in the 650 and 750 °C deformed samples is the characteristic of the C level: in DAT1 samples it is formed by two levels with different activation enthalpies ( $\Delta H = 0.37$  and 0.43 eV, respectively) but it reduces to a single line C ( $\Delta H = 0.40$  eV) in DAT3. In Figure 3 DLTS spectra referring to different dislocation densities  $N_D$  are compared: in samples with low  $N_D$ , the peaks are clearly resolved and symmetrical, while for the more deformed material, instead, the defect-state spectra are more complex, showing overlapping lines leading to asymmetrical peaks. In particular the A and C traps are visible in every spectrum, while the B and D levels clearly appear only in the

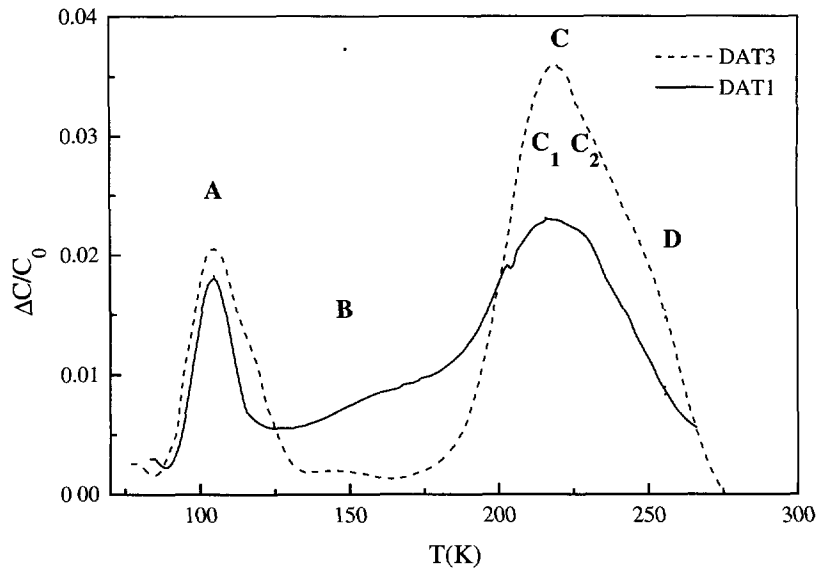


Fig. 1. — Deep Level Transient Spectroscopy spectra of DAT1 (solid line) and DAT3 (dashed line) The spectra refer to the most dislocated samples of each set (emission rate:  $e_n = 134 \text{ s}^{-1}$ , filling pulse:  $U_p = 0.3 \text{ V}$ , reverse bias:  $U_r = 7 \text{ V}$ , filling time:  $t_p = 100 \mu\text{s}$ ).

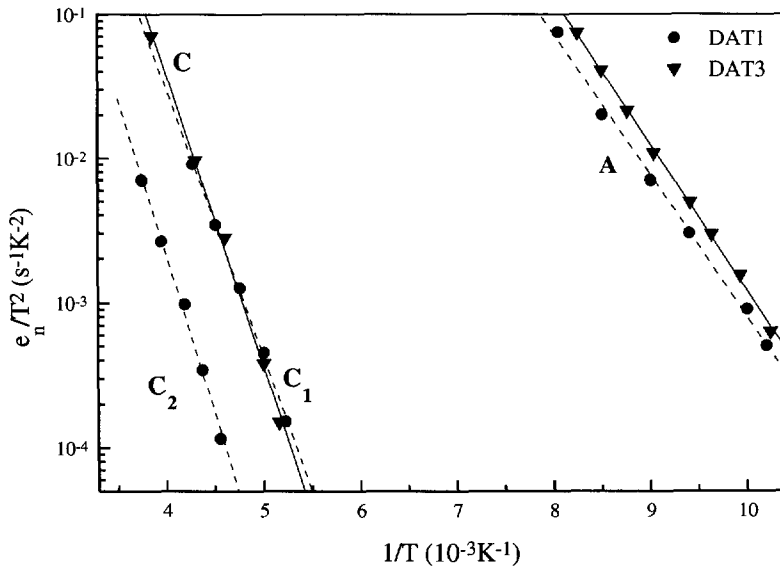


Fig. 2. — Thermal emission rates  $e_n$  ( $T^2$ -corrected) as a function of inverse temperature for the traps A, C,  $C_1$  and  $C_2$  referring to the most dislocated samples of DAT1 ( $T_d = 650 \text{ }^\circ\text{C}$ ) and DAT3 ( $T_d = 750 \text{ }^\circ\text{C}$ ) sets. The parameters of the lines A and C are reported in Table II, the ones of  $C_1$  and  $C_2$  are: activation enthalpies  $\Delta H = 0.37$  and  $0.43 \text{ eV}$  respectively, and prefactors  $A_{pf} = 8 \times 10^5$  and  $10^6 \text{ s}^{-1}$ , respectively.

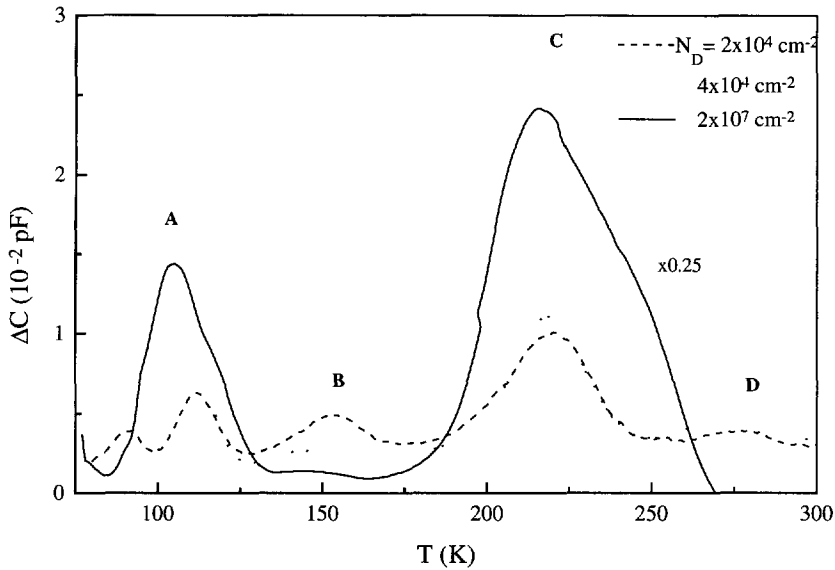


Fig. 3. — DLTS spectra of the samples with different dislocation densities of DAT3 set ( $e_n = 134 \text{ s}^{-1}$ ,  $U_p = 0.3 \text{ V}$ ,  $U_r = 7 \text{ V}$ ,  $t_p = 100 \text{ } \mu\text{s}$ ).

Table II. — Results of DLTS investigations on the less deformed sample in the DAT3 set ( $N_D = 10^4 \text{ cm}^{-2}$ ).  $\Delta H$  represents the activation enthalpy, FPHW the full peak half width of the Gaussian enthalpy distribution,  $A_{pf}$  the prefactor defined as:  $A_{pf} = \sigma_n \langle v_{th} \rangle N_{CB} \times \exp\left(\frac{\Delta S}{k}\right)$  where  $\langle v_{th} \rangle$  and  $N_{CB}$  are thermal velocity and density of states in the conduction band, respectively,  $\sigma_n$  majority carrier capture cross-section and  $\Delta S$  change in entropy due to the emission of one electron from the deep level to the conduction band.

Trap	$\Delta H$ (eV) (a)	$\Delta H$ (eV) (b)	FPHW (meV) (b)	$A_{pf}$ ( $\text{s}^{-1}$ ) (a)	$A_{pf}$ ( $\text{s}^{-1}$ ) (b)	$\sigma_n$ ( $\text{cm}^2$ ) (c)
A	0.19	0.23	0	$6 \times 10^6$	$3 \times 10^9$	
B	0.29			$2 \times 10^7$		
C	0.40	0.43	44	$5 \times 10^6$	$1.3 \times 10^8$	$8.9 \times 10^{-16}$
D	0.56			$2 \times 10^7$		

(a) Obtained from the Arrhenius plot of  $e_n/T^2$  vs.  $1/T$ .

(b) Obtained from DLTS fitting.

(c) Obtained from direct filling measurements.

samples with low dislocation density. The DLTS peak of line C is broad and built-up by non exponential transient. Consequently, the above described model of broadened deep levels has been applied. The values of the fitting parameters are reported in Table II. It can be observed that, while the line C appears to be broadened (as revealed by its FPHW value), the fitting of line A gives FPHW values close to zero (FPHW = 0 is typical for a deep level giving rise to an exponential capacitance transient). In Figure 4 the theoretical fit to the experimental spectra of the C level in samples with different dislocation densities is reported. All the C peaks have

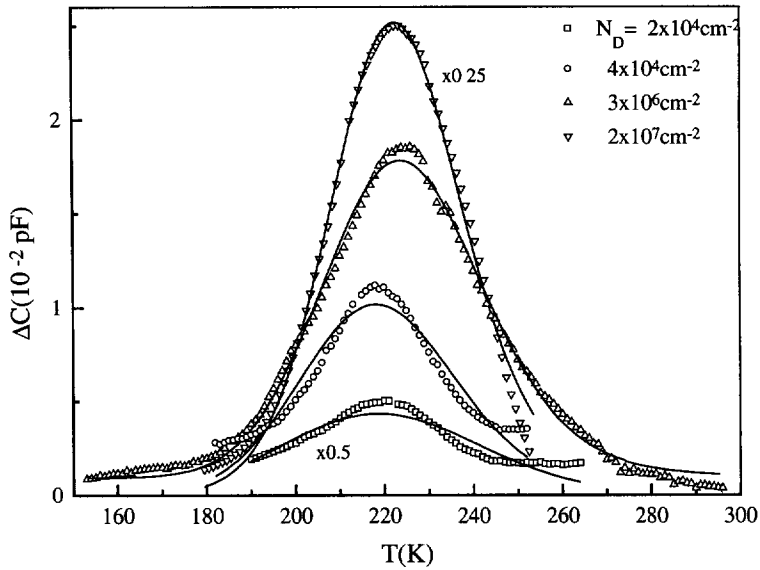


Fig. 4. — Theoretical fit to the experimental spectra of the line C in the samples with different dislocation densities of the DAT3 set ( $e_n = 134 \text{ s}^{-1}$ ). Reverse bias and filling pulse are the same as in Figure 1.

been fitted simultaneously with the same value of activation enthalpy and prefactor but with different values of line amplitudes and FPHWs. From the measured peak amplitudes and DLTS peak half widths a corrected evaluation of the density  $N_T$  of trap C has been obtained [7]. The results are reported in Figure 5: for low dislocation densities ( $N_D < 10^6 \text{ cm}^{-2}$ , range I)  $N_T$  is almost constant with respect to  $N_D$ , while for higher dislocation densities ( $N_D > 10^6 \text{ cm}^{-2}$ , range II)  $N_T$  shows a linear dependence on  $N_D$ .

The capture mechanism of the trap C has been studied in the slightly deformed specimens of set DAT3, where all the peaks were well separated. It is worth noting that the DLTS peak of trap C changes in amplitude as a function of the filling pulse width  $t_p$  holding symmetric in shape and centred at the same temperature, contrary to what observed by other authors [8]. From the plot of  $\Delta C$  vs.  $t_p$  in the range of short filling pulses ( $t_p < 10^{-5} \text{ s}$ ), where  $\Delta C$  depends on  $t_p$  according to equation (1), the cross section  $\sigma_n$  of line C has been evaluated (Tab. II). The electron density  $n_T$  captured by the C trap as a function of the filling time  $t_p$  shows a linear dependence on  $\ln(t_p)$  up to  $2 \times 10^{-4} \text{ s}$  [6]. The logarithmic capture mechanism has been modelled by a defect whose potential barrier  $\phi$  is time dependent [3]. The value of the potential barrier  $\phi$  of the C trap as a function of  $t_p$  evaluated according to this model, is shown in Figure 6. A similar behaviour has already been observed for line B and D [1], but the capture kinetics of line C has never been studied up to now.

#### 4. Discussion

DLTS is a powerful tool to investigate deep levels, however, when applied to extended defects it cannot be interpreted unambiguously. For this reason a few models [1, 8, 9] have been proposed to understand the characteristic features of DLTS spectra of extended defects, such as: i) logarithmic capture behaviour; ii) line broadening and iii) peak amplitude variation as a

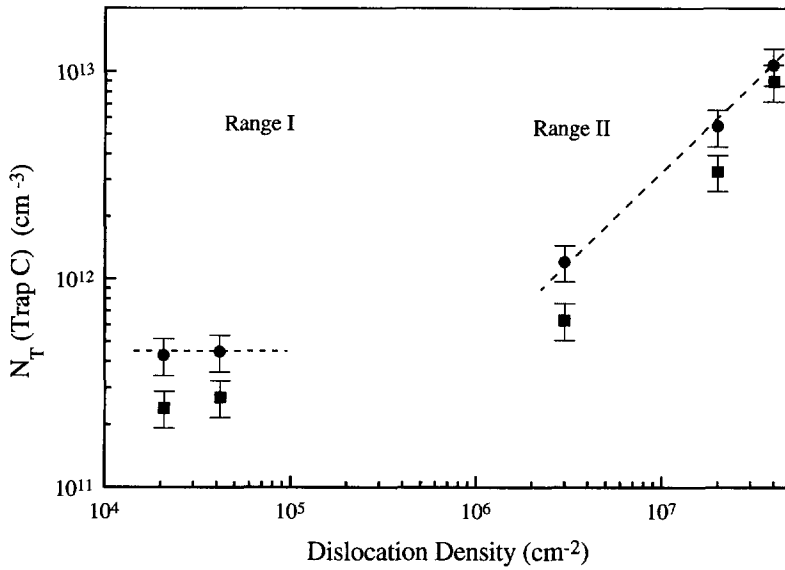


Fig. 5. — Deep level concentration of the trap C in DAT3 set as a function of the dislocation density evaluated in the conventional way (■) and corrected for line broadening (●).

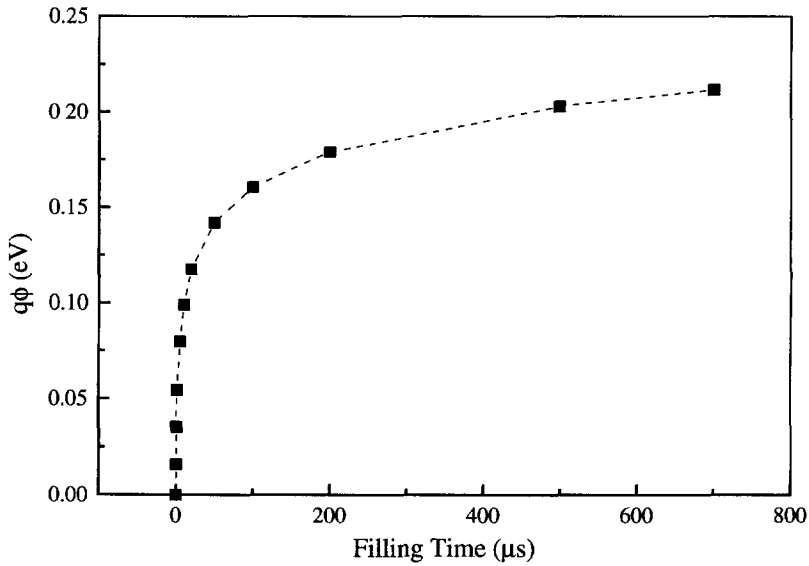


Fig. 6. — Repulsive Coulomb potential  $\phi(t_p)$  plotted vs. filling time for the C line.

function of emission rate. Referring to the present results, the logarithmic capture dependence of the peak amplitude vs. the filling pulse width  $t_p$  can be interpreted on the basis of the model for the capture kinetics reported in reference [3] which enabled us to calculate the potential barrier associated to the trap C (Fig. 6).



The peak C shows a symmetric broadening which is well fitted by the model by Omling *et al.* [7]. This model, however, does not explain the anomalous variation of the peak amplitude  $\Delta C_{\max}$  as a function of  $e_n$  which is, conversely, observed in the experimental spectra [6]. Similar effects have been observed by Grillot *et al.* [10] in strain-relaxed Si-Ge structures, by Szielko *et al.* [11] and Knobloch *et al.* [9] in PD silicon. This increase of  $\Delta C_{\max}$  *vs.*  $e_n$  could be due to different causes: i) the “ $\lambda$  volume” correction [1], which depends on temperature and causes  $\Delta C_{\max}$  to depend, in turn, on temperature, ii) a possible amphoteric behaviour of the level, which has been found to cause large variations of  $\Delta C_{\max}$  *vs.*  $e_n$  [9,12], iii) the broadening of the observed peaks [7] and iv) the temperature variation of the capture cross-section [11]. In this work these effects have been partly overcome or evaluated as, respectively, follows: i) the “ $\lambda$  volume” correction has been calculated to have only a slight effect which cannot give rise to the large variations observed, ii) the hypothesis of the amphoteric behaviour of the level cannot be applied to the present case as we observe the same effect both in the A and C levels, and both of them lie too far from the mid gap level to exhibit an amphoteric behaviour. The last two causes (iii) and (iv) are reasonably the effective ones in the present case. However, the broadening effect, evaluated according to reference [7], does not justify by itself the whole variation of the peak amplitude observed. From these findings it seems that the observed variations can be explained only if the temperature dependence of the capture cross-section is also accounted for. As a consequence an overestimation of the activation enthalpy of line C must be taken into account.

The four levels found have been related to different defects as follows. The comparison between the spectra of DAT1 and DAT3 (Fig. 1) shows that the ratio of the amplitude of DLTS peak A over the amplitude of DLTS peak C is higher in DAT1 than in DAT3, meaning that different  $T_d$ s introduce the same traps, but with different relative concentrations. A possible explanation is the following: while trap C is related to the dislocation itself, trap A is related to point defects left behind during the dislocation motion. In this respect it is worth noting that, due to the different  $T_d$ s, in DAT1 dislocations have an incubation time about two orders of magnitude higher than in DAT3 (Tab. I) and this could explain a large density of defects related to dislocation motion. Trap A increases in density with  $N_D$ , its line is never broadened and thus it could be attributed to point defects related to dislocation motion or to dislocation interaction. Traps B and D, where detected, do not show any dependence of their state density on  $N_D$ , besides, they disappear after annealing [13]. Thus they can be attributed to point defects.

Even though the line C has never been studied in detail because often masked by the more populated D line, it has been related to dislocations due to its high thermal stability [1]. Instead, the deformation procedure here used has induced defect-state spectra in which the C trap is more populated than the D one and not overlapped with it. Moreover the partial annealing of defects occurring during sample cooling reduced the contribution of B and D traps [13]. Our findings regarding the C line are the following: i) it can be separated in two peaks  $C_1$  and  $C_2$  in 650 °C deformed samples and reduces to one line in 750 °C deformed samples (Fig. 1); ii) its DLTS peak is broadened (Fig. 4); iii) it is associated to a time dependent potential barrier (Fig. 6); iv) its concentration increases with the dislocation density (Fig. 5). The first feature can be explained as follows: the peak C could be partly induced by point defects located at the dislocations, which probably anneal out during the 750 °C deformation, giving no contribution to the line C actually observed in DAT3. Both the broadening effect and the presence of a potential barrier lead to the conclusion that trap C must be related to a defect that experiences the dislocation strain field. Therefore it is localized at the dislocations. Further details regarding the differences between trap  $C_1$ ,  $C_2$  and C can be found in reference [13].

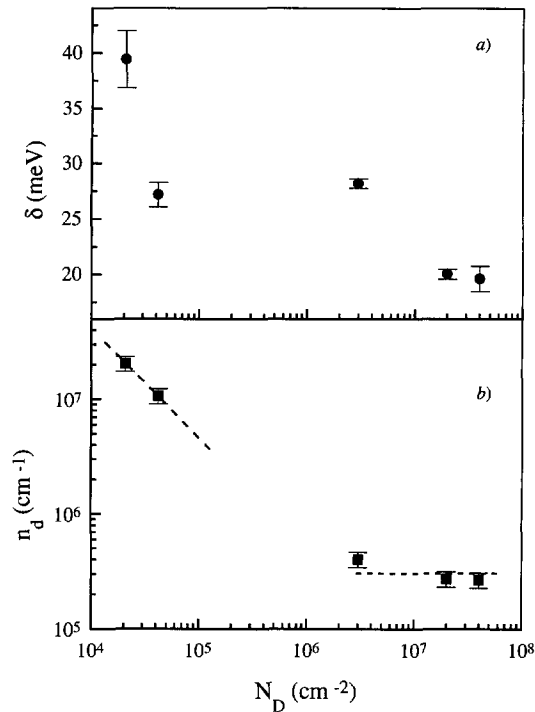


Fig. 7. — a) Broadening parameter  $\delta$  of the line C plotted as a function of the dislocation density. b) Linear state density of the line C, defined as  $n_d = N_T(\text{trap C})/ N_D$ , plotted *vs.* the dislocation density  $N_D$ . The dashed lines represent only a guide for the eye.

The broadening parameter  $\delta$  referring to line C, *i.e.* the standard deviation of the Gaussian enthalpy distribution, has been evaluated from the FPHW value. Its values are reported in Figure 7a as a function of the dislocation density. Two different physical mechanisms can be considered as responsible for the broadening phenomenon: the lattice disorder [14] and the presence of fluctuations in the potential energy occurring between different sites of randomly distributed charge defects [15,16]. The latter gives a broadening parameter which increases as a function of the total ionized defect concentration. In Figure 7b the linear state density  $n_d$  of line C (defined as  $n_d = N_T(\text{trap C})/ N_D$ ) has been reported *vs.*  $N_D$ . By observing that both  $\delta$  and  $n_d$  decrease *vs.* the dislocation density  $N_D$ , a relation between  $\delta$  and  $n_d$  can be assumed, and according to the model reported in references [15,16] it can be stated that  $\delta$  increases as a function of  $n_d$ . It follows that  $\delta$  is not simply related to the structural characteristics of a specific defect, but it is related to the defect linear charge density. The behaviour of  $n_d$  *vs.*  $N_D$  reflects the two distinct ranges of the dependence of the concentration of the trap C on  $N_D$ . Figure 5 shows that in range I ( $N_D < 10^5 \text{ cm}^{-2}$ ) the concentration of trap C does not significantly change with  $N_D$  and hence  $n_d$  slightly changes with the dislocation density. It is worth noting that: i) the values of  $n_d$  here obtained are surprisingly high; ii) in this range the dislocation distribution is strongly inhomogeneous (as found by etch pit observations). In range II ( $N_D > 10^6 \text{ cm}^{-2}$ ) the density of the level C linearly depends on the dislocation density. This further supports the attribution of the C trap to a defect localized at the dislocations. Accordingly, the linear state density  $n_d$  keeps constant in this range (Fig. 7b). This behaviour

can be explained as follows. The whole  $N_D$  range explored refers to the same set DAT3 and, consequently, the density of deformation-induced point defects is the same in each sample. A certain amount of these defects locates at dislocations giving rise to the trap C with a very high linear state density  $n_d$  in the range of low  $N_D$ . In the range of high  $N_D$  these defects rearrange themselves resulting in a significantly lower linear state density.

## 5. Conclusions

From DLTS analyses of PD silicon the four traps A, B, C and D usually found in literature have been detected. Particular attention has been paid to the DLTS line C and its broadening and capture kinetics have been studied in detail. The results concerning this line can be summarized as follows: i) its shape depends on the deformation procedure, ii) it is associated to a time dependent potential Coulomb barrier, iii) it is broadened, iv) its concentration is an increasing function of the dislocation density, v) it dominates DLTS spectra at high deformation temperature ( $T_d = 750$  °C). Therefore the trap C is undoubtedly the most closely related to dislocations among all the deformation-induced traps, while the others are mainly due to deformation induced point defects not necessarily localized at dislocations. The line broadening effect of line C has been described by the broadening parameter  $\delta$  which accounts for the disorder in the crystal. From the analysis of the behaviour of  $\delta$  as a function of the dislocation density a relationship of  $\delta$  with the dislocation linear charge density has been found.

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