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Measurements of energy spectra of extended defects

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Abstract

The density of states of two different dislocation types in silicon has been studied by computer modelling and fitting to available deep-level transient spectroscopic data. Our preliminary fit results indicate that one type, which is a dislocation bounding thin platelets consisting of two $NiSi_2(111)$ planes and supposed to be free of jogs, kinks, reconstruction defects and also point defect decoration, is associated with a one-dimensional band of states in the middle of the bandgap, 0.3 eV wide and with an electron occupation of 0.3 in the neutral state. Two fit parameters are not consistent with independent results and require the potential drop along the platelet to be incorporated in our model. For dislocations that move from a scratch under an applied stress at high temperatures, our fits, possible at present to only some of the data, show the existence of point defect clouds in the dislocation strain field and indicate the existence of core defects.

1. Introduction

Extended defects are small systems embedded in a large system, namely the semiconductor bulk. They consist of many atoms arranged in a specific structure and of many electrons with a spectrum of electronic states superimposed on the band structure of the semiconductor. A suitable way to describe this spectrum is by a density of states $N_d(E)$ (Schröter *et al* 1995).

Extended defects in semiconductors may either be infinitely extended in only one (dislocations) or two dimensions (interfaces, grain boundaries) or spatially bound in all directions (clusters, precipitates). Similar to low-dimensional nanostructures grown by deposition from the vapour phase, 1D and 2D defects are expected to act as quantum systems, if they are unperturbed. In 1D systems the electron–electron interaction leads to electronic

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excitations, which are qualitatively different from those in 3D systems (Tomonaga 1950, Luttinger 1963). Some of their properties are summarized in the article by Schönhammer (2002b).

At present only very preliminary results exist for $N_d(E)$ despite intensive research work over half a century, especially on dislocations. The analysis and interpretation of experimental data in terms of $N_d(E)$ has turned out to be impeded by two main factors: (1) the many-electron nature of extended defects and (2) their ubiquitous interaction with point defects. Point defects that segregate at the extended defect not only add a distribution of levels $N_d^{(e)}(E)$ (extrinsic spectrum) to the extended defect, but in general also destroy specific features of its intrinsic spectrum $N_d^{(i)}(E)$ (Nikolic and MacKinnon 1993, Schönhammer 2002a). Therefore experimental access to intrinsic spectra and to the specific quantum character of extended defects requires the control and, if possible, the elimination of point defects on them. This requirement is also essential for silicon technology, where for example the effect of dislocations on the minority carrier lifetime and thereby on the efficiency of solar cells is determined by their decoration with point defects.

In this paper we shall briefly review experimental efforts to obtain qualitative and quantitative features of the density of states at extended defects and of the structural features responsible for it. Criteria for deep-level transient spectroscopy (DLTS) have recently been developed which give the necessary conditions for the existence of an intrinsic or an extrinsic spectrum at extended defects (Schröter *et al* 1995). The criteria are based on the variation of the DLTS lineshape with electron filling of the defect states, measured by the filling pulse duration t_p, and categorize defect states into 'band-like' and into 'localized'. Applying these criteria to literature data, we have selected DLTS spectra in each category and have begun computer modelling and fitting to the data to determine the parameters of $N_d(E)$. We will present and discuss preliminary results.

For most extended defects the elimination of the influence of the point defect on $N_d^{(i)}(E)$ still remains an experimental challenge. In the case of dislocations, special preparation procedures for obtaining well-defined dislocations have been developed (Omling *et al* 1985, Kronewitz and Schröter 1987a, 1987b), and it has been shown, that heat treatment drastically reduces the contribution of point defects to dislocation-related DLTS (Kimerling and Patel 1979). However, our results show that even after such treatment the electrical activity of dislocations in silicon in many cases remains determined by point defects, which are positioned in the core or as clouds at the dislocation (Schröter and Cerva 2002). Very recently gettering procedures have been applied to control impurity segregation at dislocations in silicon (Kveder *et al* 2002).

Furthermore, fast quenching ($\leqslant$2000 K s^{-1}) has been used to generate very thin ($\sim$1 nm thick) $NiSi_2$ platelets with diameters between 5 and 200 nm free of point defect decoration (Seibt and Schröter 1989, Riedel and Schröter 2000). A dislocation ring, which bounds the platelet and is free of jogs or kinks, gives rise to a broadened DLTS line. According to our analysis the associated states are band-like, which is a necessary condition for an extended defect to exhibit its quantum character. Preliminary computer modelling indicates a 1D density of states, which is expected to be strongly affected by electron correlation and, if unperturbed, to be that of a Luttinger liquid (Tomonaga 1950, Luttinger 1963, Schönhammer 2002a, 2002b).

2. First energy spectra for dislocations in Ge and Si from spectral photoconductivity

In the 1970s EPR (electron spin resonance), the Hall effect and photoconductivity were the main experimental tools for investigating the electronic states of dislocations in Ge and Si. In the search for a method to determine $N_d(E)$, a modification by Mergel and Labusch (1977a, 1977b)

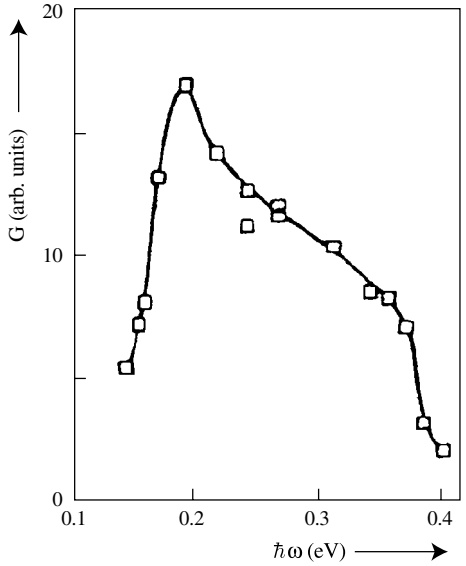

Figure 1. Effective generation yield G as a function of photon energy in p-type Ge (7.5×10^{12} cm^{-3}), deformed at 580 °C ($N_{dis} = 10^7$ cm^{-2}). A light beam parallel to the specimen axis has been used, thereby avoiding surface and contact effects on the signal $\Delta\sigma$ that are difficult to control. G is normalized to the light intensity and has been derived from the change of slope of the relative photoconductivity $\Delta\sigma/\sigma(\omega)$ on switching on the light of frequency ω (courtesy of Mergel and Labusch 1977b).

of the experimental arrangement for measuring spectral photoconductivity in connection with previous Hall data (Schröter 1967) has provided convincing evidence for a half-filled 1D band at edge-type dislocations in Ge.

In figure 1 an effective photogeneration yield G, derived from a photoconductivity measurement, is shown as a function of photon energy $h\omega$. $G(\omega)$ in fact reproduces a shape which is reminiscent of a 1D density of states. In the interpretation of Mergel and Labusch, the shape of $G(\omega)$ results from direct transitions between two 1D bands. A lower band consists of hole states that are localized in the strain field at the dislocation, while the upper band represents a half-filled band in the dislocation core. According to Hall data the upper band has an occupation limit for the neutral edge-type dislocation at 0.09 eV above the valence band edge (Schröter 1967). With this model the width of the empty part of the 1D band has been estimated by Mergel and Labusch to about 0.09 eV. These results still represent our knowledge on the electronic structure of edge-type dislocations in Ge (Schröter and Cerva 2002).

What are the results of this modified photoconductivity technique when applied to dislocation in silicon? Mergel and Labusch (1982) used their technique to study p-type Si, plastically deformed by uniaxial compression at 810 °C up to dislocation densities of several 10^7 cm^{-2}. At these temperatures ($T \geqslant 800$ °C) most the of deformation-induced point defects should quickly anneal out, so that their influence on photoconductivity should be negligible.

Mergel and Labusch found a set of full states with an upper edge at $E_v + 0.20$ eV and a set of empty states with a lower edge at $E_v + 0.50$ eV, so that the two sets are separated by an energy gap of about 0.3 eV. $G(h\omega)$ shows some features which are characteristic of a 1D band for the lower set, but not for the upper set, which the authors ascribed to a 'smeared-out group of states or even localized levels'. This means that the dislocation related density of states $N_d(E)$ in silicon contains a strong contribution from core defects or point defects located

at dislocations, which is in agreement with independent results obtained by EPR and DLTS (Schröter and Cerva 2002).

3. DLTS of extended defects

3.1. Variation of the DLTS lineshape with filling pulse duration t_p

DLTS is a powerful and well established tool for investigating deep point-defect levels. Through the registration of the capacitance transients at a Schottky contact, $\Delta C(t)$, it probes the emission kinetics of defects inside the space charge region. Since the initial occupation of defects by electrons (or holes) is adjustable by variation of the capture period preceding the emission period, the capture process of the defect is also accessible by DLTS.

For point defects, emission and capture rate, R_e and R_c, are linearly dependent on the electron occupation of the defect level, so that $\Delta C(t)$ is exponentially dependent on time during capture and emission. Then, to determine the electrical parameters of a point defect, one investigates the variation of the position of the line maximum with registration frequency ν_r and filling pulse duration t_p. As a fingerprint, which is useful for identifying the defect by comparison with available data found in handbooks (Schröter and Seibt 1999), the emission rate as a function of temperature $e_n(1/T)$ is frequently used.

Only a few years after its first application to point defects, plastically deformed silicon has also been studied by DLTS (Kimerling and Patel 1979). The spectra consist of several overlapping lines, which reduce to two on annealing at $T \geqslant 800\,^{\circ}\mathrm{C}$: the C line in n-type silicon and the F line in p-type silicon (Kveder *et al* 1982). Both are significantly broader than the lines associated with point defects and also show different emission and capture kinetics. Although certain qualitative aspects like the effect of the dislocation line charge on the capture kinetics were soon realized, a quantitative analysis to determine a density of states or levels is still missing. Until recently the DLTS data for dislocations (and other extended defects) were analysed in the same way as those for deep point defects. The only modification was the introduction of a Gaussian distribution of point defect levels (Omling *et al* 1985). This analysis simply attributes some formal 'effective' energy level and capture cross section to the dislocation, which—as has been shown recently by computer simulations (Hedemann and Schröter 1997b)—have no clear relation to the real density of states at dislocation.

When one goes to formulate the emission and capture rate of an extended defect, R_e and R_c, with consideration of $N_d(E)$ one encounters two problems:

(i) R_e is a superposition of the emission rates of the occupied states belonging to $N_d(E)$. But the occupation of each single state is determined by two processes, by the capture of electrons from the conduction band during the previous capture period and by the internal electron exchange between the defect states. So far this problem, which would need the introduction of internal exchange rates, has not been solved. However, for two limiting cases R_e can easily be calculated if the effect of the internal electron exchange is approximated by an internal equilibration time Γ_i (see figure 2(a)) ((Schröter *et al* 1995)). Γ_i is defined as the time it takes to arrange the distribution of captured electrons into a Fermi distribution with a quasi-Fermi level characterizing the non-equilibrium occupation. Then the two limiting cases are given by $\Gamma_i \ll R_e^{-1}$ and $\Gamma_i \gg R_e^{-1}$. In the first case the internal exchange rate is large and the defect states have been called 'band-like', in the second they have been named 'localized' or simply 'levels'.

(ii) The second problem arises from the effect of the electrostatic potential of the defect on the capture rate R_c. This effect has been taken into account by a capture barrier δE_e impeding the electron transition from the conduction band to the defect. δE_e depends on

the total electrostatic charge of the extended defect, which is the sum over the occupation of all states of $N_d(E)$. The occupation of each energy state is the result of its electron capture and its electron emission, with its capture rate modified by the effect of δE_e, which depends in turn on the occupation of all states. This is a complication which generates a tough problem for computer calculations: one has to solve a system of strongly coupled nonlinear rate equations where each of them describes the time evolution of occupation of states $N_d(E)$ in the energy range from E_i to $E_i + \mathrm{d}E$. Since the energy step $\mathrm{d}E$ should be chosen small enough to describe the spectrum $N_d(E)$ properly, the number of equations can be quite large for a broad energy spectrum.

3.2. Physical models for the two cases $\Gamma_i \ll R_e^{-1}$ and $\Gamma_i \gg R_e^{-1}$: silicide platelets and dislocations in silicon

Possible candidates for band-like states ($\Gamma_i \ll R_e^{-1}$, see figure 2(a)) are the unperturbed internal states of extended defects, e.g. those of the 1D bands at dislocations or of 2D bands at grain boundaries or interfaces, while a set of levels ($\Gamma_i \gg R_e^{-1}$, see figure 3(a)) coupled by a common capture barrier could result from point defects inside the extended defects, e.g. jogs, kinks or reconstruction defects in the dislocation core, or from impurities segregated in their long-range strain field, like point defect clouds at dislocations.

With variation of the filling pulse duration t_p, the DLTS lineshape has been found to develop in one of two different ways (see figures 2(b) and 3(b)). It has been shown that the defect parameter which controls this t_p-dependence is the electron equilibration time Γ_i (Schröter *et al* 1995).

Spectra with small Γ_i values ($<10^{-5}$ s) have been found for thin $NiSi_2$ and Cu_3Si platelets (thickness ~1 nm, diameter 7–200 nm) (Sattler *et al* 1998) and also for small spherical Cu_3Si platelets.

DLTS lines of the type shown in figure 3(b), whose amplitude ΔC varies approximately according to $\Delta C \sim \ln(t_p)$, have been found in deformed n-type Si (Patel and Kimerling 1979). Some of them disappear on annealing at 800°C. The one shown in figure 3(b) survives and is associated with 60° dislocations (C line). Γ_i is now large so that internal equilibration can be neglected during DLTS. The extended defect states behave like point defect levels, but the occupation of each level is coupled to that of all other levels. Possible candidates for this type of spectrum are defects in the dislocation core or point defect clouds, which form in the dislocation strain field. First fits to experimental data have been based on the model of a point defect cloud as shown in figure 3(a).

The above DLTS analysis makes it evident that a t_p dependence of the lineshape is the fingerprint of an extended defect similar to $e_n(1/T)$ for point defects. In other words, to extract the information about $N_d(E)$ and the nature of states ('band-like' or 'localized') from DLTS it is necessary to analyse the dependence of the DLTS lineshape and position not only on frequency but also on t_p.

4. Computer modelling

4.1. Computer modelling of the $NiSi_2$ platelet electronic structure

It has been demonstrated by computer simulations that thin $NiSi_2$ and Cu_3Si platelets, as obtained by fast quenching (~2000 K s^{-1}) from diffusion temperatures, possess a spectrum of band-like states (Schröter *et al* 1995, Sattler *et al* 1998). $NiSi_2$ platelets fit almost perfectly into the silicon lattice. They consist of two $NiSi_2(111)$ planes embedded into silicon and connected

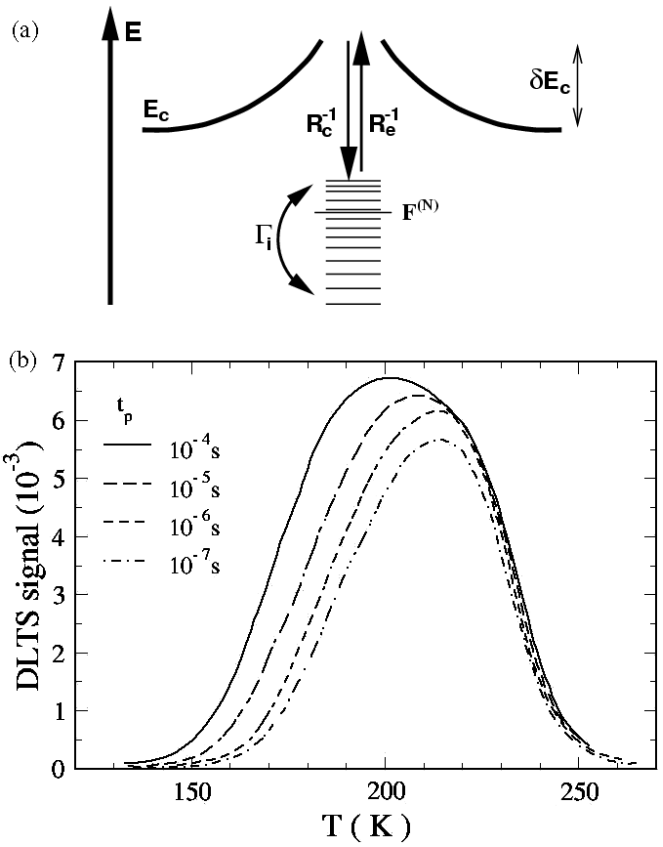

Figure 2. (a) Electronic model of an extended defect with 'band-like' states ($\Gamma_i \ll R_e^{-1}$) used for computer simulations of DLTS (Schröter *et al* 1995). (b) DLTS curves as a function of the filling pulse duration t_p of $NiSi_2$ platelets, consisting of two (111)$NiSi_2$ layers in n-type silicon (1.4×10^{15} cm^{-3}): $v_r = 68$ Hz, bias voltage = 4 V, pulse voltage= 4 V (courtesy of Riedel and Schröter (2000)).

to Si(111) planes by Si–Si-bonds, so that all Ni atoms except those at the rim are sevenfold coordinated instead of eightfold in bulk $NiSi_2$ (Seibt and Schröter 1989).

The absence of dangling bonds at the interface requires a relative shift of the two Si shores, which then has to be compensated at the rim of the platelet by a dislocation of the Burgers vector $\boldsymbol{b} = (a/4)\langle 111\rangle$ (Seibt and Schröter 1989). The diameter of the thin platelets can be controlled by variation of the diffusion temperature and quenching rate to between a few nanometres to almost 1 μm (Seibt and Schröter 1989, Riedel 1994). This means that the core of the dislocation, which bounds the platelet, offers a highly effective reaction channel for incorporation of interstitial nickel atoms into a growing $NiSi_2$ precipitate. Platelets and dislocations form a system that is self-adjusting to strict planar extension. As a consequence, the dislocation core does not contain jogs and kinks. Its curvature results from defects which have been called 'joints'. In a ball-and-stick model (Seibt and Schröter 1989, Riedel and Schröter 2000), a dislocation core has been constructed which is free of silicon dangling bonds but contains Ni atoms with sixfold and fourfold coordination as a possible source of electrical activity. The joints differ from the core only by a fourfold coordinated Ni atom replacing a fivefold coordinated one. The number and coordination of the Si atoms, the periodicity, and

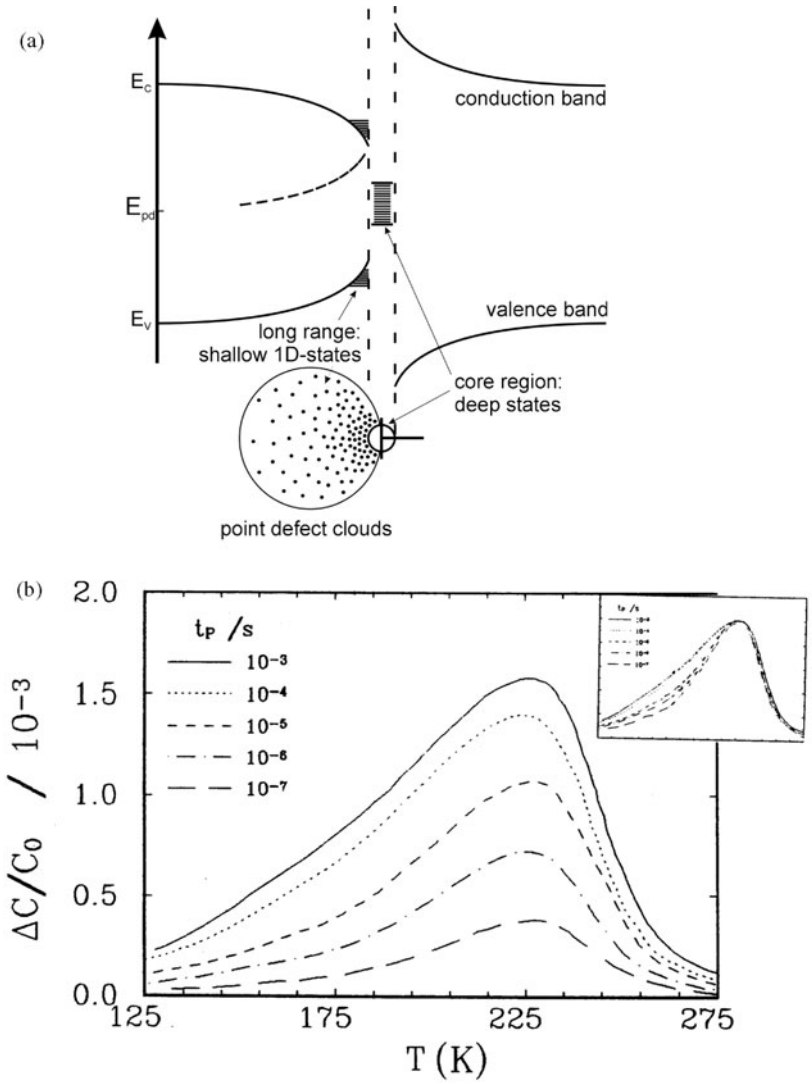

Figure 3. (a) Electronic model of a point defect cloud at a dislocation giving rise to localized states ($\Gamma_i \gg R_e^{-1}$) used for computer simulations of DLTS (Schröter *et al* 2002). (b) DLTS lines as a function of t_p for 60° dislocations (dislocation density from etch pit counting: 4×10^6 cm^{-2}) in n-type (4.5×10^{14} cm^{-3}) silicon. Bias voltage = 4 V, pulse voltage = 4 V, $\upsilon_r = 17$ Hz (Kronewitz (1986), courtesy of Kronewitz and Schröter (1987a, 1987b).)

the back bonds remain unchanged. Riedel and Schröter (2000) argue that as a consequence joints should only weakly perturb the 1D electronic system at the core, comparable to the meandering of quantum wires in heterostructures (Nikolic and MacKinnon 1993).

In this structural model, $NiSi_2$ platelets are composed of two types of extended defect, interface and dislocation, both without silicon dangling bonds and with under-coordinated Ni atoms in their cores. Compared with more compact precipitates the platelets are not stable due to a larger surface energy and larger energy of the dislocation bounding the platelet. The $NiSi_2$ grows in the form of platelets instead of more compact precipitates owing to a

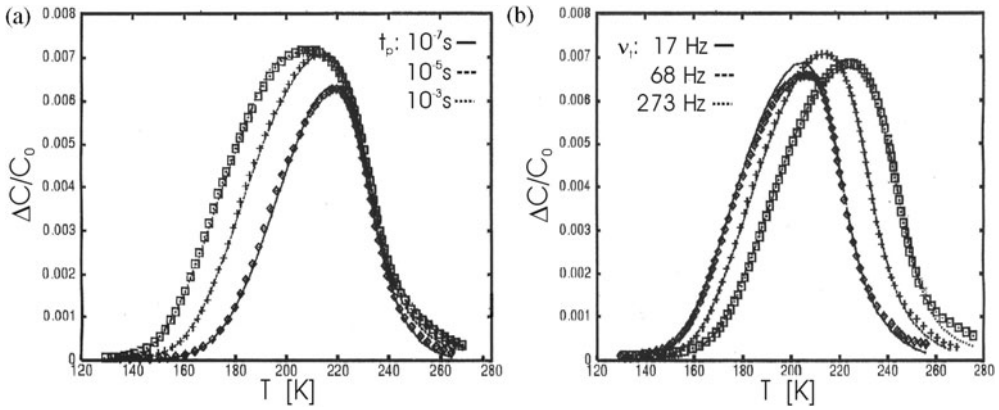

Figure 4. Simultaneous fit of a 1D density of states (free parameters: band edges, $E_c - E_1 = 0.42$ eV and $E_c - E_2 = 0.71$ eV, and occupation in the neutral state $F^{(N)} \approx 0.33$) to DLTS-data (registration frequency $\upsilon_r = 68$ Hz: $t_p = 10^{-7}$, 10^{-5}, and 10^{-3} s; $t_p = 10^{-5}$ s: $\upsilon_r = 17, 68,$ and 272 Hz), obtained for $NiSi_2$ platelets having a diameter of 37 ± 6 nm in n-type silicon (P concentration 1.4×10^{15} cm^{-3}, in-diffusion of Ni at 900 °C, quenching rate ∼2000 K s^{-1}). The capture barrier has been taken as $\delta E_c = \alpha(F - F^{(N)})$ with the free parameter $\alpha = 0.72$ eV. Electron and hole emission have been considered with the capture cross section as free parameters: $\sigma_n = 5 \times 10^{-14}$ cm^2 and $\sigma_p = 5 \times 10^{-15}$ cm^2. The field effect has been described by an effective point charge as free parameter: $q^* \approx 2.7$.

very effective growth mechanism via bounding dislocation, achieving fast relaxation of a highly supersaturated Si–Ni solid solution. Still unresolved is the question of the nucleation of the platelet, since dislocations have a large self-energy of several electron-volts per core period. This is part of the general, still unsolved problem, of how homogeneous nucleation of dislocations is achieved.

On annealing around 300 °C, the platelets undergo an inner transformation to a more compact shape, and, at the same time, their DLTS line characteristics change from the band-like type to the localized type. From a careful comparison of the structural changes observed by HREM, with the electronic change, Riedel and Schröter (2000) concluded that the energy spectrum giving rise to the DLTS line of $NiSi_2$ platelets has its origin in the dislocation bounding the platelet. In their model, a transformation of the 1D band to localized states occurs due to generation of a large number of core defects at the bounding dislocation during a structural transformations. In 1D system, defects can easily destroy the original 1D energy band, making electronic states localized.

Starting with a simple 1D density of states, we have made a computer model of the platelet electronic structure. So as not to lose the physical significance of the model, we tried to keep the number of free parameters sufficiently small to arrive at a critical check of the model by comparing its results with experimental data and even to make predictions whose incompatibility with experiment could lead to modifications of the model. By this strategy, physical parameters which are relevant for the description of the experimental data are distinguished from those that are of secondary importance.

To determine its free parameters, we performed a fit of the model simultaneously to six DLTS spectra measured in a wide range of t_p (10^{-3}, 10^{-5} and 10^{-7} s) and registration frequencies ($\upsilon_r = 17, 68$ and 273 Hz), so that the parameters are relevant for all spectra within those ranges. The result is presented in figure 4 where the experimental data are shown by symbols, while lines show the fitted theoretical spectra calculated for a 1D density of states. The agreement is very good.

To obtain such a good fit it was necessary to take into consideration the following points:

(1) When the 1D band includes very deep states (equal to or deeper than about half of the bandgap of silicon) hole emission has to be considered as a possible process in addition to electron capture and emission.
(2) To prove the relevance of hole emission, Hedemann and Schröter (1997a) investigated the Poole–Frenkel effect, i.e. the effect of an electric field on the emission both experimentally and theoretically. The main contribution from field enhancement of emission was attributed to the strain field of the bounding dislocation. Its effect on the conduction band leads to a shift of the low- T side of the DLTS line, that on the valence band to a shift of the high- T side. In the experiment both shifts occurred, so that $NiSi_2$ platelets behave as recombination centres. Those authors also showed that the Poole–Frenkel effect of $NiSi_2$ platelets shows approximately the same temperature and field dependence as a point charge with 3D Coulomb potential, so that an effective point charge q^* may be used as a model parameter.

The curves shown in figure 4 are the results of the fit using a 1D density of states with the following values of the free parameters: upper and lower band edges $E_c - E_1 = 0.42$ eV and $E_c - E_2 = 0.71$ eV, occupation of states in the neutral state $F^{(N)} \approx 0.33$, the parameter α used for calculation of capture barrier $\delta E_c = \alpha(F - F^{(N)})$ is $\alpha = 0.72$ eV, electron and hole capture cross sections $\sigma_n = 5 \times 10^{-14}$ cm^2 and $\sigma_p = 5 \times 10^{-15}$ cm^2, effective point charge $q^* \approx 2.7$ and total number of states $N_{tot} \approx 2 \times 10^{14}$ cm^{-3}.

A very surprising result of our fit is the small total number of states N_{tot}. The original idea was to assume that a possible source of electrical activity in dislocations bounding $NiSi_2$ platelets are Ni atoms with sixfold and fourfold coordination. Using transmission electron microscopy (TEM) the density and size of the platelets were determined, and from these the density of fourfold and sixfold coordinated Ni-atoms in the core of the bounding dislocation was estimated as $N_{\mathrm{Ni(4)}} = N_{\mathrm{Ni(6)}} = 2.2 \times 10^{15}$ cm^{-3}. This value is about 10 times larger than the total number of states $N_{tot} \approx 2 \times 10^{14}$ cm^{-3} obtained from the fit.

Another point which is also not quite understood at the moment is the large value of the parameter q^*. There are four sets of $\{111\}$ platelets, all having the same angle with the Schottky contact (100) plane, and six possible Burgers vectors for each set (Hedemann and Schröter 1997a). For these various combinations of dislocation line elements and Burgers vector, the calculations yield q^* values between 0.7 and 1.2 for electron emission and between 0.9 and 1.5 for hole emission. One can see that the value of q^* obtained from a fit is at least two times larger than the estimated values.

In summary, experimental DLTS data for the $NiSi_2$ platelets can be quite well described by a theoretical model assuming the existence of a 1D energy band of width 0.3 eV with a filling in the neutral state of 0.3. This energy band can be attributed to the dislocation bounding the platelet. However, there are still some unanswered questions and some weak points in our present modelling. The most intriguing result is the surprisingly small total density of states N_{tot} in this band, obtained from a fit, which is about 10 times smaller than the density of under-coordinated Ni-atoms in the dislocation core derived from TEM-data. One of the weak points is the way we have treated the effect of the external electric field on $N_d(E)$. We have used the rigid band model for a mean value of the electric field over the platelet and have neglected the variation of it along the platelet. For a typical value of $F = 5 \times 10^4$ V cm^{-1} the potential drop along the platelet (diameter 37 nm) is about 0.2 eV, so that its electrical parameters can vary significantly from one end to the other. Recently, two problems arising from this variation have been analysed by one of us (Hedemann 2002). It has been shown that the potential drop is sufficiently small on the atomic scale to justify presentation of the

platelet's electronic states by a coherent $N_d(E)$. Regarding the emission rate, however, the quasi-Fermi distribution function has to be replaced by an integral over the dislocation ring, whose implementation into the fitting program leads to unacceptable computation times and requires the development of approximations suitable for fast computation. This problem is unresolved at present.

4.2. Dislocations in Si: the defects behind the C line

The prominent DLTS line in plastically deformed n-type silicon, which survives after annealing at 800 °C, is a line measured in the T range between 150 and 250 K. Compared with the line of a point defect, it is considerably broadened.

Looking at the results of different authors, the C line does not have a clear identity. Variation of the lineshape with t_p is common (see below), but the shape itself varies from strongly asymmetric (Kronewitz 1986, Kronewitz and Schröter 1987a, 1987b, Birkner 1994) to nearly symmetric (Cavalcoli *et al* 1997a, 1997b), and the reason for this variation is not clear at present. Recently, a strong influence of metallic impurities such as Ni, Cu, and Au on the electrical activity of dislocations has been demonstrated. The electron beam induced current (EBIC) contrast of dislocations between 50 and 300 K has been quantitatively explained using a model, that assumes electron–hole recombination to be controlled by the coupling between deep impurity levels and shallow 1D bands at dislocations (Kveder *et al* 2001). Furthermore, a large increase in the DLTS signal in the range of the C line was observed, when Ni was diffused into plastically deformed silicon (Kveder *et al* 2002). Subsequent Al gettering led to a reduction of that DLTS signal to below that of the C line, as observed directly after plastic deformation.

Some authors have found evidence that in the temperature range where the C line is observed, two broad lines, C_1 and C_2, occasionally appear, with the C_2 line lying at higher temperatures than the C_1 line (Omling *et al* 1985). The C_2 line has its maximum at about the same position as the C line, while the C_1 line has its maximum at the low-T side of the C line. Recent investigation by Knobloch *et al* (2002), who applied DLTS and scanning DLTS to $Si/Si_{0.98}Ge_{0.02}$ heterostructures (grown by chemical vapour deposition at 1080 °C on Si(100)-substrates), have shown that gold segregated at the misfit dislocations is associated with a broadened line at the position of the C_1 line and of similar shape. They also found that the broadening of their DLTS line increases with increasing decoration by gold, as estimated from the EBIC contrast of the dislocation.

In what follows, we take for the C line the one observed by Kronewitz (1986) and by Birkner (1994). The development of the shape of the C line with the filling pulse duration t_p is significantly different from that for the $NiSi_2$ platelets described in section 4.1. As the main features valid for localized states, $\Gamma_i \gg R_e^{-1}$, the position of the line maximum stays almost constant within a large t_p-range and the maximum and the high-T side of the line are related to t_p by $\Delta C_m(T \geqslant T_{max}, t_p) \sim \ln(t_p)$ (see figure 3(b)).

Therefore the states giving rise to the C line are localized and must come from point defects at dislocations, either in its core or segregated in its strain field or both. The broadening of a core level is expected to result from fluctuating fields (electric (Figielski 1990) or elastic (Kisielowski and Weber 1991)) and should give a moderately and symmetrically broadened DLTS line, whose line amplitude ΔC_m still follows $\Delta C_m \sim \ln(t_p)$.

Computer simulations of DLTS have been performed previously for a point defect cloud in the strain field of an edge-type dislocation on the basis of the model shown in figure 3(a) (Schröter *et al* 1995). For the simulations the density of point defects has been assumed to be constant within a small cylinder (radius ∼1 nm) touching the dislocation core. The generated

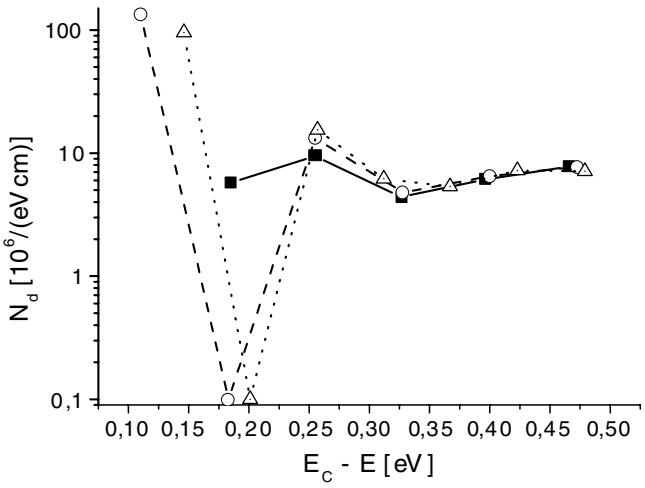

Figure 5. Density of levels as obtained from a simultaneous fit to the DLTS data presented in figure 3(b) for $t_p = 10^{-7}$, 10^{-6}, and 10^{-5} s. ■: fit parameters: $N_d(E)$ represented by five density-values, upper edge $E_c - E_1 = 0.185$ eV and lower edge $E_c - E_2 = 0.466$ eV, capture cross section $\sigma_n = 5.8 \times 10^{-16}$ cm^2, and dislocation density $N_{dis} = 3.8 \times 10^6$ cm^{-2}. ○: $N_d(E)$ by six values, $E_c - E_1 = 0.11$ eV, $E_c - E_2 = 0.473$ eV, $\sigma_n = 7.9 \times 10^{-16}$ cm^2, $N_{dis} = 3.8 \times 10^6$ cm^{-2}. △: $N_d(E)$ by seven parameters, $E_c - E_1 = 0.146$ eV, $E_c - E_2 = 0.479$ eV, $\sigma_n = 9.8 \times 10^{-16}$ cm^2, $N_{dis} = 3.8 \times 10^6$ cm^{-2}. Please note the good agreement between the N_{dis} values and those obtained from etch pit counting (see figure 3(b)).

DLTS lines are indeed asymmetrically broadened, their maxima and high-T sides increase proportionally to $\ln(t_p)$, but the low-T side is much too steep compared with the C line, as measured by Kronewitz (1986) and by Birkner (1994). It has been argued that a rearrangement of the point defects inside the cylinder by elastic interaction might correct this discrepancy (Schröter and Cerva 2002). In addition, a core defect could contribute to the C line. To check these possibilities, we have recently begun computer modelling with the aim of determining the density of states $N_d(E)$ in a parametric form from a fit of a suitable dislocation model (see figure 3(a)) to available data for the C line.

We present $N_d(E)$ for a set of localized states (levels) without intrinsic electronic exchange between them. For each of the energy levels we solved the rate equation valid for point defects, but with a modification of the capture rate to account for the effect of the electrostatic potential of the dislocation line charge. This potential has been calculated for different screening mechanisms by Read (1954) and by Schröter and Labusch (1969) and we took their results (see also Labusch 2002). As one of the free parameters of the model we take the dislocation density N_{disl}, which may also be considered as a control parameter since it is has also been measured by the etch pit technique. To represent $N_d(E)$ we have used as free parameters the upper and lower edge position with respect to the conduction band edge, and five, six or seven values of the density of states at equally spaced energy values including the band edges.

The algorithm used for fitting only works for a short filling pulse $t_p \leqslant 10^{-5}$ s, which limits the simultaneous fit to only three lines out of the five that have been measured (see figure 3(b)). The results for density of states $N_d(E)$ obtained by the fit are shown in figure 5. A much more effective algorithm has recently been developed but not yet implemented into the program. Therefore the results which are shown in figure 5 have to be considered as preliminary.

The dislocation densities N_{dis} resulting from the fit agree pretty well with those obtained from etch pit counting (see figure 3(b)).

The densities of states $N_d(E)$ represented by five (figure 5: ■), six (figure 5: ○) (or seven (figure 5: △)) values are quite similar for deep states, when $(E_C - E) > 0.25$ eV. In this energy range $N_d(E)$ yields a continuous curve and its shape is close to the distribution which can be expected for a point defect cloud collected by dislocations due to their elastic interaction with point defects. $N_d(E)$ for such a cloud can be described by a formula that has a clear physical meaning and includes three parameters (Schröter and Cerva 2002): one is the point defect level in the bulk $E_c - E_{pd}$, the other two contain combinations of the point defect level shift with strain, given as a deformation potential Ξ_{pd}, the temperature T_{diff}, at which the point defects are still sufficiently mobile to respond to the interaction with the dislocation, the point defect misfit ε, and the total concentration of segregated point defects. Note that deformation potentials of point defects Ξ_{pd} have been measured independently using the stress dependence of the emission rate $e_n(p, 1/T)$ (Feichtinger and Prescha 1989).

For energies $(E_C - E) < 0.25$ eV, the fitted $N_d(E)$ first drops down and then again increases (see figure 5). This could indicate that in addition to the point defect cloud, dislocations have some other, shallower states, possibly associated with their core. However, our present results are very preliminary and some more experiments and computer modelling are still necessary to come to any final conclusions about the real physical nature of dislocation related states observed by DLTS.

5. Conclusions

In summary, previous measurements of the spectral photoconductivity have given first evidence of a deep 1D band at dislocations in Ge and in Si. For both materials this band is positioned in the lower half of the semiconductor bandgap. In silicon, a further set of localized states, was found 0.3 eV above the upper edge of the 1D band.

With DLTS an important fingerprint of electronic states at extended defects comes from the variation of the lineshape with filling pulse duration, which allows us to classify the states as 'band-like' or as 'localized'. Going a step further, we have described our efforts to derive parameters of the density of states, $N_d(E)$, at dislocations in Si from modelling the emission and capture characteristics of dislocations and simultaneous fits to DLTS lines, measured for wide ranges of registration frequency and filling pulse duration.

For small dislocation loops (diameter ∼37 nm) at the rim of thin $NiSi_2$ platelets we obtained a partially filled 1D band about 0.3 eV wide and positioned around the middle of the silicon energy gap. However, two fit parameters, the total density of states N_{tot} and the effective charge q^*, differ significantly from their measured and estimated values respectively. Both discrepancies indicate that the field effect needs to be treated more carefully.

As an example for localized states, we have considered the C line, which has been found to be associated with 60° dislocations in Si and is observed as an isolated line after careful annealing at $T \geqslant 800\,^{\circ}$C. To model $N_d(E)$ we have taken two parameters for its width and position in the bandgap and another five, six or seven parameters to simulate the shape of $N_d(E)$. The experimental DLTS data cover a range of filling pulse durations 10^{-7} s $\leqslant t_p \leqslant 10^{-3}$ s. However, limitations in our present program allow simultaneous fitting to only three spectra measured for $t_p \leqslant 10^{-5}$ s. Our preliminary results show clear evidence for the existence of a point defect cloud at 60°-dislocations in silicon.

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