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Dislocation-related electroluminescence at room temperature in plastically deformed silicon

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Dislocation-related photoluminescence and electroluminescence properties have been studied in heavily dislocated silicon crystals between about 2 K and room temperature. A model explaining the high-temperature stability of the $D1$ luminescence is suggested and considerations concerning the nature of the $D1$ centers are presented. The experimental results are in good agreement with these models. In particular, forward-biased diodes exhibited an intense structureless luminescence band at 1.55 μm which clearly originated from the $D1$ centers.

I. INTRODUCTION

Light emission from silicon-based devices has recently attracted considerable attention, though undoped silicon due to the indirect energy gap is expected to exhibit only very weak luminescence properties. The indirect band gap implies that recombination of electrons and holes involve optical phonons of momentum equal to the difference Δp of the momentum for holes and electrons. In order to increase the quantum efficiency of luminescence in silicon it is therefore advisable to find proper methods for excluding phonons from recombination processes. This can, for example, be achieved by channeling the recombination of charge carries via deep electronic states. Among impurity centers with large binding energy, rare-earth-related centers have already shown very promising results.[1] Other centers which are of interest in this context are deep states originating from intrinsic defects such as dislocations.

The dislocation-related photoluminescence (DRL) in Si is known to consist of four lines (or bands) which are labeled $D1$ (0.81 eV), $D2$ (0.87 eV), $D3$ (about 0.95 eV), and $D4$ (about 1.0 eV),[2] and have been investigated quite extensively.[3–6] Experiments with so-called low-temperature-high stress (LTHS) plastic deformation[7] show that the energy positions of $D3$ and $D4$ strongly depend on the distance d between partials in dissociated perfect dislocations.[5,8] LTHS results in a considerable dispersion of d for different dislocations with the same orientation. Since $d = an$, where a is a lattice parameter in the [112] direction and n is an integer, the large dispersion of d leads to a splitting of the $D3$ and $D4$ bands into a number of lines.[8] The energy positions of these lines, $E(n)$, are well described by the phenomenological expression[9] $E_n = E_\infty - A'\exp(an/b)$. Using these results, the authors of Refs. 8, 9, and 10 concluded that the $D3$ and $D4$ bands originate from recombination processes at straight segments of 60° dislocations. In addition, it has been suggested[10] that the $D3$ line most probably is a phonon-assisted replica of $D4$.

At high dislocation densities, the $D1$ line is dominant with respect to the photoluminescence (PL) intensity. The intensity of this line is less affected by temperature than the intensity of the other lines since the binding energy of the ground state involved in the luminescence is larger in this case than for other lines. Also, the energy position of the line is of technological interest since it coincides with the absorption minimum in silica-based glass fibers.

The origin of $D1$ and $D2$ is, compared with $D3$ and $D4$, less clear. Stacking faults between dislocations, impurity atoms in the strain field around dislocations, and dislocation jogs and segments of dislocations of special types (like lomer dislocations) are typical examples for the origin of the $D1$ and $D2$ lines suggested in the literature.

The purpose of this paper is to investigate different possibilities for a considerable increase of the quantum efficiency of the dislocation-related luminescence in silicon. For reasons which will become clear later we focused our interest on the $D1$ line, with the intention of further clarifying the nature of the line.

II. EXPERIMENTAL DETAILS

Samples $4\times4\times12$ mm^3 in size were cut from p-type floating zone (FZ) Si doped with 3×10^{15}-cm^{-3} boron. The samples were 10–15 % plastically deformed at $T = 1050\,^\circ$C by compression along [123]. Platelets with a thickness of about 1 mm were cut from the central parts of the deformed samples for diode fabrication. In order to decrease the concentration of nonradiative intrinsic defects, additional annealing at 1100 °C was performed. All treatments were carried out under clean conditions in a N_2 or Ar atmosphere with the intention to avoid metal contamination.

Two different methods were used for fabricating diodes. In the first case a small pellet of gold, doped with Sb, was placed on a silicon wafer. The wafer was then heated to a temperature slightly higher than the eutectic temperature ($=400\,^\circ$C) resulting in a heavily doped n region between the pellet and the wafer. In the second case, the emulsitone emitter diffusion source $N250$ was used in order to form phosphorus-doped SiO_2 on the wafer surface. The samples were covered with the $N250$ solution and then baked at 125 °C for 50 min in air. Afterwards, the samples were annealed at 1100 °C for 60 min in a N_2 or argon ambient. The mesa structures were

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fabricated by wet etching. A Ga-Al alloy was used for providing Ohmic contacts to the p-type substrate, whereas Al wires were bonded to the n-type layer.

The photoluminescence and electroluminescence (EL) spectra were recorded with a spectral resolution of 3 nm using standard lock-in techniques in conjunction with a Jobin-Yvon HRD1 grating monochromator and a North Coast germanium diode as a detector. The measurements were performed in a variable-temperature cryostat with electrical feedthrough in the temperature range 1.9–300 K. The PL was excited by the 514-nm line of an Ar-ion laser in the power range between 0.1 and 100 mW/mm, whereas the EL was generated by applying a forward bias to the diodes.

III. RESULTS

Deep-level transient spectroscopy (DLTS) measurements were performed on diodes fabricated in plastically deformed p-type samples as well as in n-type samples in order to find out whether or not deep electronic traps were present. No dislocation-related DLTS peaks[11,12] were monitored. Depending on the sample, various DLTS signals were observed corresponding to trap concentrations less than 10^{13} cm^{-3}. Arrhenius plots of thermal emission rates obtained from such studies resulted in activation energies which were close to known values of Fe- and Mo-related centers[13,14] as well as Cu-B pairs[15] in p-type and to P-V complexes in n-type[16] samples.

At low temperatures ($T < 20$ K) our samples exhibited typical dislocation-related PL spectra implying that the $D1$, $D2$, $D3$, and $D4$ lines were clearly detected. The solid curve in Fig. 1(a) shows the PL spectrum of sample $K3$ at $T = 5$ K. In heavily deformed samples, the intensity of the $D2$, $D3$, and $D4$ lines decreased very quickly with increasing temperature and at $T > 40$ K only the $D1$ band was observed [dashed curve in Fig. 1(a)]. All data discussed below are related to this band.

At low excitation density, the half-width dE of the PL band depended very weakly on temperature, as shown by the open squares in Fig. 2(b). The solid curve is given by $dE = 33.5$ meV$+0.5kT$ and is therefore clearly different from the dependence $dE = 33.5$ meV$+3kT/2$ which is expected in the case of optical transitions between a three-dimensional (3D) energy band and deep energy levels [dashed line 1 in Fig. 2(b)]. The weaker dependence of dE on T implies that the $D1$ luminescence is best understood in terms of optical transitions between two localized states rather than between the conduction or valence band and localized states. The measured energy positions of the $D1$ PL band as a function of temperature is exhibited by open squares in Fig. 2(a). The solid curve 1 in Fig. 2(a) shows the calculated temperature dependence $E_g(T) - 362$ meV, where $E_g(T)$ is the energy gap of silicon at temperature T. Evidently, at low excitation density the energy positions of the $D1$ band follows rather well the temperature dependence of E_g. If it is assumed that the $D1$ band originates from optical transitions between two localized energy states, these states have energies $E_v + E_{D1v}$ and $E_c - E_{D1c}$, where $E_{D1c} + E_{D1v}$ is about 362 meV.

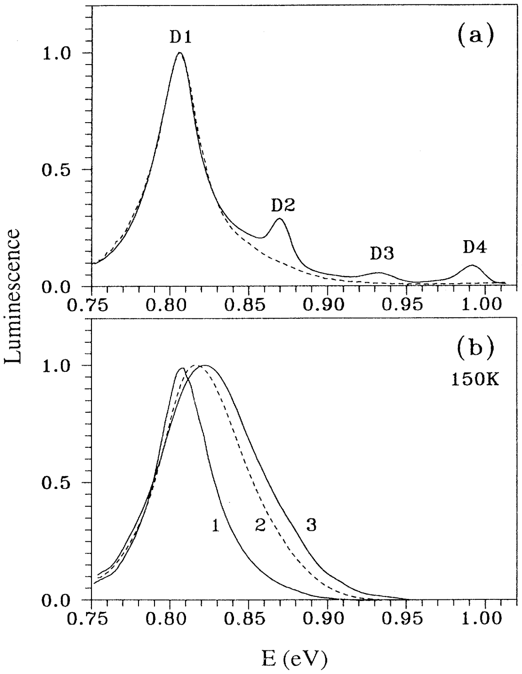

FIG. 1. (a) Normalized photoluminescence (PL) spectra of sample $K3$ at $T = 5$ (solid curve) and 50 K (dashed curve). The Ar-laser excitation density was 6 mW/mm^2. (b) normalized spectra of sample $K3$ at $T = 150$ K for different excitation densities: Curve 1: Ar laser, 20 mW/mm^2; curve 2: electroluminescence (EL) spectrum, current density 100 mA/mm^2; curve 3: EL spectrum, current density 400 mA/mm^2. The energy scale is shifted by $E_g(0\text{ K}) - E_g(150\text{ K})$, where $E_g(T)$ is the energy gap of Si at temperature T.

At low current density j ($j < 10$ mA/mm^2), the electroluminescence (EL) spectra exhibit a spectral distribution similar to the PL spectra, but at higher current densities $D1$ becomes broader and its maximum shifts to higher energies [Fig. 1(b)]. The energy shift and the half-width of the EL band are proportional to $\ln(j)$ [Fig. 3(a)]. The broadening of the EL band cannot be explained by saturation effects since, as one can see from Fig. 3(b), the EL intensity AdE depends almost linearly on j ($AdE \approx j^{(0.8 \text{ to } 0.9)}$). Curve 2 in Figs. 2(a) and 2(b) shows the temperature dependence of the $D1$ energy positions and its half-width for a diode current of $j = 400$ mA/mm^2. Both the additional broadening and energy shift at low temperature, caused by the high excitation level, decreased with increasing temperature and approached the PL data.

The temperature dependence of the luminescence amplitude A is shown in Fig. 4. Curves 1 and 2 correspond to the EL signal from two different diodes at a current density of 400 mA/mm^2, whereas the curve labeled PL corresponds to the PL signal obtained with a laser excitation of 100 mW/mm^2. The EL efficiency of the diode, fabricated according to method 1 (curve 1) is almost ten times lower than the one of the diode, which was structured using the multitone emitter diffusion source (curve 2).

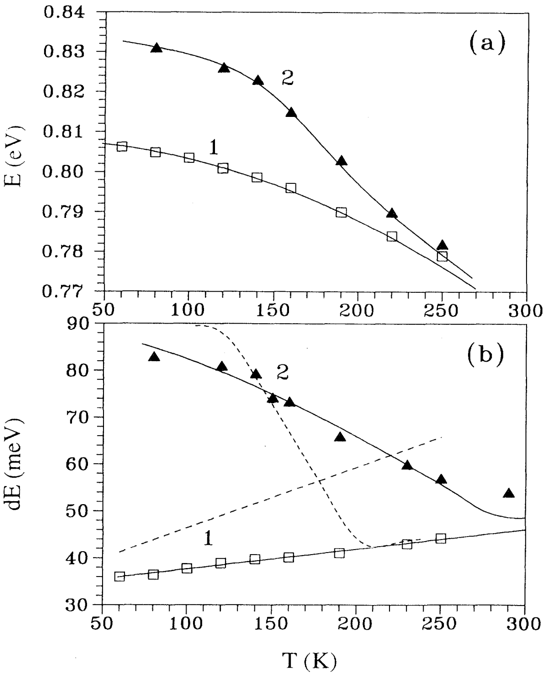

FIG. 2. Temperature dependence of the energy position $E(T)$ and half-width $dE(T)$ of the $D1$ band. Curve 1: Ar-laser excitation, 20 mW/mm^2; curve 2: electroluminescence, diode current density 400 mA/mm^2.

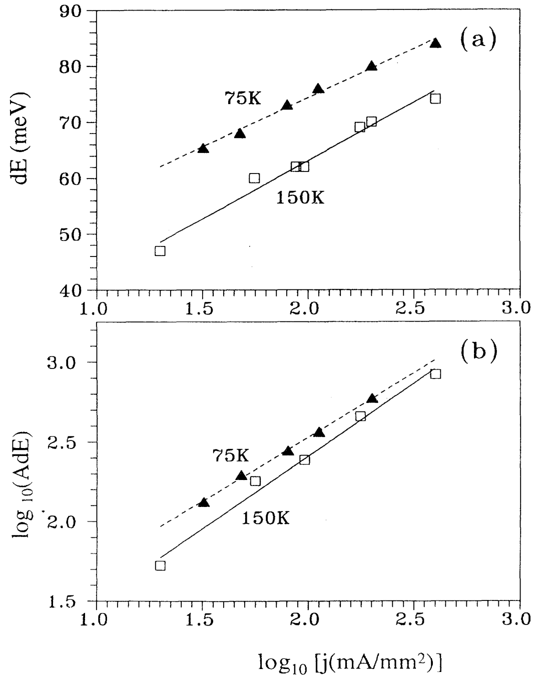

FIG. 3. (a) Dependence of the half-width dE of the $D1$ EL band on diode current density j. (b) Dependence of the EL intensity AdE on j.

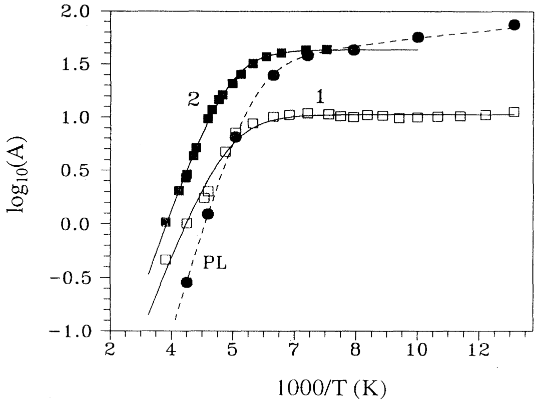

FIG. 4. Temperature dependence of the $D1$ band amplitude of sample $K3$. Curve 1: EL of the diode fabricated by diffusion of Sb from Au/Sb alloy, diode current 100 mA; curve 2: EL of the diode fabricated by P diffusion from P_2O_5, diode current 50 mA; PL curve: Ar-laser excitation, 100 mW.

IV. DISCUSSION

As already mentioned in Sec. III, the weak temperature dependence of dE observed at low excitation density could imply that the $D1$ luminescence originates from internal transitions of a defect center and, hence, that the center has two energy levels: E_v+E_{D1v} for holes and E_c-E_{D1c} for electrons.

The solid and dashed curves in Fig. 4 have been calculated using the relation

$$A(T)=B/[1+CT^3/2\exp(-E_A/kT)]\ , \tag{1}$$

which is often applied to describe the occupation of deep electronic states by electrons or holes. C and B are temperature independent coefficients. The activation energy E_A often differs very little from the binding energy of the deep state. From the best fitting we found that the activation energy E_A should be about 0.15 and 0.16 eV for curves 1 and 2, respectively, and that the corresponding energy for the PL curve was 0.17 eV. A still better fitting to the PL curve is obtained if B is assumed not to be temperature independent but to be proportional to T^{-1}. If it is assumed that the activation energy E_A corresponds to E_{D1v} or E_{D1c} then, taking into account that $E_{D1c}+E_{D1v}$ is about 362 meV, one has to conclude that E_{D1c} and E_{D1v} are almost equal, i.e., both should have values of about 150–200 meV.

This result is not in agreement with the data obtained in Ref. 4, reporting on the temperature dependence of the $D1$, $D2$, $D3$, and $D4$ lines in FZ p-Si samples plastically deformed by 2% at 900 °C. The authors of Ref. 4 found that the PL amplitude is indeed well described by Eq. (1), but they obtained deactivation energies of 7 meV for $D1$ and about 4 meV for the $D2$, $D3$, and $D4$ lines. In heavily dislocated Si, deformed at 750–850 °C, the authors of Ref. 5 obtained a similar temperature dependence, though with a deactivation energy E_A for $D1$ of about 10 meV. In all samples used in Refs. 4 and 5, the intensity of the dislocation-related PL lines, including $D1$, began to decrease quickly for $T > 30$ K, whereas in our samples a substantial decrease was only observed for $T > 140$ K.

Before we discuss this discrepancy in more detail we need a better understanding of the following observations: (1) the broadening and energy shift of the $D1$ band at high excitation, and their dependences on T and j; (2) the much higher thermal stability of the $D1$ luminescence compared with the $D2$, $D3$, and $D4$ bands; and (3) the absence of DLTS signals originating from E_{D1c} and E_{D1v}, at least in the temperature range from 77 to 300 K.

If E_{D1c} and E_{D1v} are energy levels corresponding to point defects randomly distributed in the bulk, the results discussed so far are difficult to explain. The model we prose to explain our observations is therefore based on the following assumptions.

(1) The centers responsible for the $D1$ band are not randomly distributed point defects but probably defects on dislocations. We assume that centers responsible for the $D2$ and $D4$ luminescence are also connected to dislocations.

(2) A distribution of $D1$ energy levels exists due to a possible variation of the local strain and electric field. The hole level $E_v + E_{D1v}$ of the $D1$ center therefore varies within the range $E_v + E_{\max}$ and $E_v + E_{\min}$.

(3) The linear density N_t of $D1$ defects along a dislocation is larger than $1\text{–}2 \times 10^6\ \text{cm}^{-1}$.

Figure 5 shows schematically the energy diagram of our model in the direction along the dislocation. The $D1$ centers are the deepest energy states in our model, both with respect to electrons and holes. The model anticipates that redistribution of holes between the $D1$ centers is possible not only via the valence band E_v, but also by thermal excitation to dislocation-related energy states above some energy E_m (mobility edge), implying that in this case holes can move along the dislocation in the 1D energy band. A similar situation is anticipated for electrons.

The exponential decrease of luminescence with increasing temperature, observed for $T > 200$ K (Fig. 4), indicates that the recombination of electrons and holes at centers, responsible for the $D1$, $D2$, $D3$, and $D4$ luminescence, is not the main recombination channel, but that some other nonradiative recombination centers must exist and that the recombination of free carriers occurs mainly via these nonradiative centers, at least at high temperatures. We assume that in our samples these nonradiative recombination centers are not found at dislocation segments which give rise to the $D1$, $D2$, $D3$, and $D4$ luminescence, but that they are either located at some other dislocations or generated by point defects in the vicinity of these dislocations. Nonradiative centers of high concentrations at dislocations which are responsible for the D lines will be analyzed below, when possible reasons for the small activation energy of the $D1$ luminescence reported in Refs. 4 and 5 are discussed.

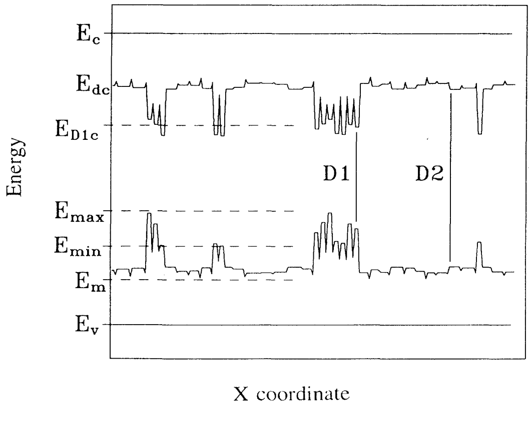

FIG. 5. Schematic energy diagram of heavily dislocated silicon.

Since the dislocation density N_D is high in our samples (about $3 \times 10^9\ \text{cm}^{-2}$), it is assumed that the lifetime τ_e of the free electrons is rather short and that the concentration of electrons n therefore is not very high. For example, if the electron capture radius of dislocations, r, is assumed to be more than 1 nm, the electron lifetime $\tau_e \approx (v_e r N_D)^{-1}$ is shorter than 3×10^{-10} s, where v_e is the thermal velocity of electrons. An Ar-laser excitation density of 100 mW/mm^2 and, hence, an electron-hole generation rate G of about $10^{23}\ \text{cm}^{-3}\,\text{s}^{-1}$ is therefore expected to result in a free-electron concentration $n = G\tau_e$ of less than about $5 \times 10^{13}\ \text{cm}^{-3}$.

In an EL experiment the density of nonequilibrium electrons is higher. The current through the diode is given approximately by $j = en(D/\tau_e)^{1/2}$, where D is the diffusion constant of electrons. Assuming an electron mobility μ of about 1000 cm^2/V s and using the relation $D = kT\mu/e$, a value of about $5 \times 10^{14}\ \text{cm}^{-3}$ is obtained for n at $j = 100\ \text{mA/mm}^{-2}$. This concentration is less than the concentration of free holes $p = 3 \times 10^{15}$ cm. The absence of near-band edge luminescence, i.e., free excitons (FE's), electron-hole drops (EHD's), and bound excitons (BE's) further supports our assumption of a large recombination rate.

For simplicity, it is assumed that recombination occurs only when electrons and holes are present at the same center, i.e., when electron-hole pairs exist. The pair decomposition time due to the thermal dissociation of electron-hole pairs is given by $[N_c v_e \sigma_e \exp(-E_{D1c}/kT) + N_v v_h \sigma_h \exp(-E_{D1v}/kT)]^{-1}$, where $N_c = N_{c0} T^{3/2}$ and $N_v = N_{v0} T^{3/2}$ are the effective states in the conduction and valence bands, respectively. Assuming that the capture cross sections σ_e and σ_h of $D1$ centers for electrons and holes are of the order of $10^{-14}\ \text{cm}^2$, the decomposition time is calculated to be about 10^{-10} s at 300 K for $E_{D1c} = 0.16\text{–}0.2$ eV. Later, we will assume that the pair lifetime is always shorter than the decomposition time due to the thermal activation of electrons or holes and, hence, that the pair lifetime is smaller than 10^{-10} s–10^{-11} s.

With these assumptions, the rate R of electron-hole recombination via $D1$ center equals the rate of pair formation since electrons and holes will always recombine as soon as they meet at the same $D1$ center (at least for $T < 300$ K). Recombination via $D1$ centers can be either radiative or nonradiative. The $D1$ luminescence intensity is therefore equal not to R but to αR, where α is the fraction of radiative recombination with respect to the total recombination at $D1$ centers. α is a characteristic parameter of the center and probably does not depend strongly on temperature. The luminescence intensity A should therefore be proportional to αR, which is given by

$$\alpha R = \alpha(n v_e \sigma_e P + p v_h \sigma_h N + \beta N P) \ . \tag{2}$$

Here p and n are the concentrations of free holes and nonequilibrium electrons, v_e and v_h are thermal velocities of free electrons and holes, and N and P are the linear densities of electrons and holes trapped to $D1$ centers. The first term in the brackets describes the generation of e-h pairs due to the capture of free electrons into the $D1$ centers which are already occupied by holes. The second term stems from the trapping of free holes onto $D1$ centers already occupied by electrons. The third term describes the formation of a pair due to the movement of already trapped electrons and holes along the dislocation, i.e., from one $D1$ center to another. β may depend on the temperature in our model.

The statistics for the occupation of dislocation-related centers differ from the one for point defects not only due to the ability of trapped carriers to move along the dislocation without excitation into the band, but also due to the fact that the trapped carriers cause a Coulomb band bending $e\phi$ around the dislocation which is given by

$$e\phi = 2e(P\text{-}N)\{\log_{10}[(P\text{-}N)L_r] - 0.4\}/\varepsilon \ , \tag{3}$$

where ε is the dielectric constant and L_r is the screening length (we assume $P > N$). Since $e\phi$ should always be less than E_{D1v} we choose $e\phi = 0.16$ eV and obtain a value of about 10^6 cm^{-1} for P-N. If therefore the density of the $D1$ center is larger than 10^6 cm^{-1} and $N < N_t$ (weak illumination), only a part of the $D1$ centers will be occupied by holes even at very low temperature. Hence in thermal equilibrium centers responsible for the $D2$, $D3$, and $D4$ luminescence are expected to be empty since they are shallower than $D1$. With increasing illumination density $e\phi$ becomes smaller and can be calculated taking into account that the total flow of electrons to dislocations must be equal to the flow of holes. At high excitation densities when n is comparable to p, $e\phi$ can be neglected.

Summarizing these considerations, one obtains

$$dP/dt = p v_h \sigma_h (N_t - P - N)\exp(-e\phi/kT) - n v_e \sigma_e P - P N_v v_h \sigma_h \exp(-E_{D1v}/kT) - \beta N P \ , \tag{4}$$

and, hence, in the steady state,

$$P \approx p v_h \sigma_h (N_t - N)\exp(-e\phi/kT) + [n v_e \sigma_e + p v_h \sigma_h \exp(-e\phi/kT) N_v v_h \sigma_h \times \exp(-E_{D1v}/kT) + \beta N]^{-1} \ . \tag{5}$$

The corresponding expression for N is

$$N \approx n v_e \sigma_e (N_t - P) \times [n v_e \sigma_e + p v_h \sigma_h \exp(-e\phi/kT) + N_c v_e \sigma_e \exp(-E_{D1c}/kT) + \beta P]^{-1} \ . \tag{6}$$

Substituting N and P into Eq. (2), the luminescence intensity is calculated self-consistently. Since N is small compared with N_t in the excitation range used in our measurements, P can also be neglected in comparison with N_t. At higher temperatures, βNP in Eq. (2) should decrease with increasing temperature with an activation energy $E_{D1c} + E_{D1v} \approx 0.36$ eV. Since a much smaller activation energy of about 0.14–0.17 eV has been observed experimentally for A, this term can obviously be neglected in Eqs. (2), (4), and (6) for temperatures above 150–200 K. It should be noted that the product NP in Eq. (2) can also be neglected at sufficiently high temperatures since NP decreases much faster with increasing temperature than N and P. With these assumptions the equation for the luminescence intensity reduces to

$$A = B/[1 + C_h T^{3/2}\exp(-E_{D1v}/kT)] + B/[1 + C_e T^{3/2}\exp(-E_{D1c}/kT)] \ , \tag{7}$$

where

$$B \approx \frac{\alpha p n v_e v_h \sigma_h \sigma_e N_t \exp(-e\phi/kT)}{[n v_e \sigma_e + p v_h \sigma_h \exp(-e\phi/kT)]} \ ,$$

$$C_e = N_{c0} v_e \sigma_e / [n v_e \sigma_e + p v_h \sigma_h \exp(-e\phi/kT)]$$

and

$$C_h = N_{v0} v_h \sigma_h / [n v_e \sigma_e + p v_h \sigma_h \exp(-e\phi/kT)] \ .$$

Furthermore, N_c and N_v have been replaced by $N_{c0}T^{3/2}$ and $N_{v0}T^{3/2}$, respectively. In the case of EL measurements, when n is probably larger than 10^{14}–10^{15} cm^{-3}, $e\phi$ is smaller than 30 meV. At $T > 150$ K $\exp(-e\phi/kT)$ is therefore a very slow function of T and B, and C_e and C_h can be considered nearly constant, implying that Eq. (7) is almost identical to Eq. (1), which has been used for the fitting of our experimental data shown in Fig. 4.

It is difficult to decide which of the energies E_{D1c} or E_{D1v} in Eq. (7) should be attributed to the energy E_A obtained from the best fitting of the experimental data. Since, however, the obtained value of E_A is about half of the sum $E_{D1c} + E_{D1v}$, this could imply that $E_{D1c} \approx E_{D1v}$.

Supposing the second term in Eq. (7) is larger than the first one, it is readily seen that E_A is mainly determined by the slope of the Arrhenius plot at high temperatures, whereas C is determined by the temperature at which the fast decrease of the luminescence starts. In this region, $v_h \sigma_h p \exp(-e\phi/kT)$ is of the order of $n v_e \sigma_e$ giving $n \approx N_{c0}/2C$. Hence dividing N_{c0} by C values obtained from the best fitting of Eq. (2) to our experimental data, n values of about 0.5×10^{15} and 1×10^{15} cm^{-3} are obtained for curves 1 and 2 in Fig. 4. In these cases, $e\phi \approx kT \ln(p/n)$ is about 25 and 10 meV at about 200 K, implying that the temperature dependence of $\exp(-e\phi/kT)$ can indeed be neglected compared with the fast change of A (see Fig. 4).

The $N_{c0}/2C$ value obtained from our photoluminescence studies is estimated to be close to 5×10^{13} cm^{-3}, resulting in a value of about 60 meV for $e\phi$. This implies that $e\phi$ can no longer be neglected compared with E_{D1v} and E_{D1c}, and it is therefore not possible to use Eq. (1) instead of Eq. (7) for describing the temperature dependence of A. The values estimated for n from the parameter C are nevertheless of the right order of magnitude. This means that the model proposed for the temperature dependence of the luminescence is self-consistent.

We will now discuss the half-width dE of the $D1$ luminescence band in more detail. Let us assume that the excitation level is so low that the distribution of the holes between the $D1$ centers corresponds to the thermodynamic equilibrium. In this case, only the deepest $D1$ centers are occupied due to the Coulomb limitation $P<N_t$. The shallower $D1$ centers as well as all $D2$ and $D4$ centers are empty. This means that only energy levels from $E_v+E_{\max}$ to $E_v+E_{\max}+P(E_{\max}-E_{\min})/N_t-kT$ are occupied by holes, and only centers with energies in this interval will contribute to the luminescence.

Any local field which shifts the hole level E_{D1v} should also shift the electron level E_{D1c} of the center. In order to evaluate the influence of the local field on the electron level and, hence, on the energy of the luminescence transitions, we assume that a shift δE_{D1v} of E_{D1v} causes a shift of the electron level by $\delta E_{D1c}=\gamma\delta E_{D1v}$. The luminescence band width can then be approximated by

$$\delta E\approx(1+\gamma)[P(E_{\max}-E_{\min})/N_t+kT]\ . \qquad (8)$$

Considering that we obtained $dE=33.5$ meV$+0.5kT$ of the photoluminescence band of $D1$, it is reasonable to assume that γ is about -0.5. Hence, if the hole level is shifted closer to the valence band by δE_{D1v}, the electron level is also shifted to lower energy, but only by about $0.5\delta E_{D1v}$, which implies a shift of the luminescence to higher energy by $0.5\delta E_{D1v}$.

During excitation of the luminescence, there is a permanent flow of electrons and holes toward dislocations. The electron flow is given by $nv\sigma_eN_m$, which prevents the hole distribution from obtaining thermodynamic equilibrium since holes are captured into any of the dislocation centers, independent of their energy. At low temperature, the average waiting time of holes on a dislocation prior to recombination is about $1/nv\sigma_e$. During this time, holes can relax to deeper energy states. The relaxation process includes thermal excitation of holes from E_v+E_{D1v} to the mobility edge E_v+E_m (see Fig. 5) as well as the drift to another center and subsequent trapping. The time needed for such processes is roughly given by $\exp[(E_{D1v}-E_m)/kT]/(v\sigma_hN_m)$, where N_m is the effective density of states at the mobility edge E_m. It is then possible to define a critical energy E_{th} in such a way that holes trapped on a center of energy $E_{D1v}=E_{\text{th}}$ have a thermal excitation time into the mobility edge which is equal to its recombination time:

$$\exp[(E_{\text{th}}-E_m)/kT]/(v\sigma_hN_m)=1/nv\sigma_e\ .$$

The distribution of holes between the centers with an energy in the range from E_v to E_{th} will then roughly correspond to the thermodynamic equilibrium, whereas centers deeper than E_{th} will be randomly occupied. For small excitation densities such that $E_{\text{th}}>P(E_{\max}-E_{\min})/N_t$, dE is still given by Eq. (8) and does not depend on the excitation level. If the excitation is so high that $E_{\text{th}}<E_{\min}$, then the luminescence band is given by $dE=(1+\gamma)(E_{\max}-E_{\min})$. In intermediate cases, the width dE is given by $(1+\gamma)(E_{\max}-E_{\text{th}})$ or

$$dE\approx(1+\gamma)(E_{\max}-E_m+kT\ln[n\sigma_e/N_m\sigma_h)+kT]\ . \qquad (9)$$

At moderate excitation densities, n is proportional to the excitation level and, hence, $n\sigma_e/N_m\sigma_h=Sj$, where S is a proportionality factor implying that dE should increase proportional to $\ln(j)$ in agreement with the experimental results presented in Fig. 3(a).

Another observation which should be discussed is the dependence of dE on T at high excitation levels [curve 2 in Fig. 2(b)]. It is readily shown that fair agreement of all experimental data with Eq. (7) is obtained by assuming $\gamma\approx-0.3$ and $E_{\max}-E_m\approx0.13$ eV, which confirms that the dependence of dE on the temperature and excitation level is reasonably understood within the model. $E_{\max}$ should have a value close to $E_A+dE/2(1+\gamma)$ and it is therefore assumed that $E_{\max}$ is about 0.2–0.21 eV. The good agreement of Eq. (9) with our experimental data suggests a value of about 0.06–0.08 eV for E_m. The dashed curve 2 in Fig. 2(b) shows the calculated temperature dependence of dE with the assumptions $E_{\max}=0.21$ eV and $E_m=0$.

Still, Eq. (9) is only a rough approximation and does not take into account, for example, the real energy distribution of the centers and the possible dependence of E_m on T. Nevertheless, the estimated energy E_m agrees well with the bottom of the 1D energy band E_v+E_{dv} which has been attributed to the regular parts of 60° dislocations[17,18] and studied by measurements of microwave conductivity.

According to Refs. 8, 10, and 19, the $D3$ and $D4$ PL band are most probably connected with the 1D energy bands E_v+E_{dv} and E_c-E_{dc} corresponding to regular parts of the 60° dislocations. Our results are then best understood with the assumption that the $D1$ centers correspond to distinct positions on these dislocations, such as jogs and constrictions or segments of other dislocation types. At very low temperatures, for example at 5 K, redistribution of holes between different $D1$ center is not possible by exciting them from E_{D1v} to E_m. Nevertheless, at low excitation, the width of the $D1$ band is smaller than its maximum width. This means that, in addition to the hole redistribution channel, discussed above, another channel must exist which makes the hole transfer between $D1$ centers possible without exciting them to E_{dv} or E_v bands. This channel is probably not as efficient as the first one at high temperature, but should dominate at low temperatures due to the very small activation energy.

To explain the low-temperature hole (or electron) transfer between $D1$ centers, we assume that the $D1$ centers form clusters and that tunneling between centers within a cluster is possible. This suggestion seems to be obvious considering that the $D1$ centers correspond to extended defects like long jogs, constrictions, or segments of other dislocation types.[19]

In general, the regular parts of dislocations are not very long and, at very low temperatures, the carriers in the 1D bands are localized between defects of the dislocation core. However, the energy barriers originating from these defects are probably not very high and a thermally activated movement of carriers along the dislocation network is possible. If the percolation radius along the dislocation network is larger than the thickness of the depletion region of the diodes used for DLTS measurements, no DLTS signal from dislocation-related centers is expected since carriers can leave the depletion region without excitation to the 3D band. This is one of the possible explanations for not observing any DLTS signal due to $D1$ centers in our samples.

Applying this explanation further, we can easily explain the very small activation energies obtained in Refs. 4 and 5 for the $D1$, $D2$, $D3$, and $D4$ lines compared with our results for the $D1$ line. In our model, the $D2$ and $D4$ centers are not the deepest energy levels on the dislocations, implying that the activation energies of the $D2$, $D3$, and $D4$ lines correspond to the excitation of electrons and holes from the $D2$, $D3$, and $D4$ centers to the mobility edge of the dislocation-related 1D energy band. The activation energy of this excitation is rather small and the $D2$, $D3$, and $D4$ PL lines disappear therefore rather quickly with increasing temperature since all carriers are trapped at deeper centers (in our case, at $D1$). The excitation of electrons and holes from the $D1$ centers to the $1D$ band as well as the movement of carriers along the $D1$ cluster (see Fig. 5) do not result in a drastic decrease of the luminescence in our case due to the low concentration of other deep recombination centers at the dislocations. Only excitation of electrons and holes from $D1$ centers to 3D energy bands results in a strong decrease of the total luminescence intensity. In our samples, the deactivation energy of the $D1$ luminescence therefore corresponds to the excitation of electrons from the $D1$ energy levels to the 3D bands, which is rather large, whereas the deactivation energies of the $D2$, $D3$, and $D4$ luminescence bands correspond to the excitation energy of electrons (or holes) to the 1D energy bands, which are rather small and comparable to those obtained in Refs. 4 and 5.

The low activation energy of the $D1$ luminescence obtained in Refs. 4 and 5 is understood if it is taken into account that the samples in Refs. 4 and 5 have been deformed at much lower temperatures than in our case. DLTS (Refs. 11 and 12) and electron paramagnetic resonance (EPR) measurements have shown that deep nonradiative recombination centers are generated at dislocations at low deformation temperatures. The lower the deformation temperature, the higher the concentration of these deep centers. Using EPR data, some of them have been attributed to dangling bonds. In this case, the excitation of electrons (and holes) from $D1$ centers to any local mobility edge, resulting in a movement of carriers along the dislocation, is accompanied by a decrease of luminescence since the carriers will be trapped to dangling bonds and other deep nonradiative centers. This means that the activation energy of the $D1$ luminescence as well as the $D3$ and $D4$ luminescence in Refs. 4 and 5 probably corresponds to the activation of charge transfer along the dislocation resulting in trapping of carriers to nonradiative centers. The activation energy of this process is much smaller than the one necessary for activation of carriers to 3D bands.

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[1] H. Ennen, G. Pomrenke, A. Axman, K. Eisele, W. Haydl, and J. Schneider, Appl. Phys. Lett. **46**, 381 (1985).

[2] N. A. Drozdov, A. A. Patrin, and V. D. Tkachev, Pis'ma Zh. Eksp. Teor. Fiz. **23**, 651 (1976) [Sov. Phys. JETP Lett. **23**, 597 (1976)].

[3] M. Suezawa and K. Sumino, Phys. Status Solidi A **78**, 639 (1983).

[4] M. Suezawa, Y. Sasaki, and K. Sumino, Phys. Status Solidi A **79**, 173 (1983).

[5] S. Sauer, J. Weber, J. Stolz, E. R. Weber, K.-H. Kürsters, and H. Alexander, Appl. Phys. A **36**, 1 (1985).

[6] V. Higgs, E. C. Lightowlers, and S. Tajbakhsh, Appl. Phys. Lett. **61**, 1087 (1992).

[7] K. Wessel and H. Alexander, Philos, Mag. **35**, 1523 (1977).

[8] R. Sauer, Ch. Kisielowski-Kemmerich, and H. Alexander, Phys. Rev. Lett. **57**, 1472 (1986).

[9] A. N. Izotov, A. I. Kolyubakin, S. A. Shevchenko, and E. A. Steinman, Phys. Status Solidi A **130**, 193 (1992).

[10] E. A. Steinman, Proceedings of the 17th International Conference on Defects in Semiconductors 17 [Mater. Sci. Forum **143-147**, 537 (1994)].

[11] J. R. Patel and L. C. Kimerling, Cryst. Res. Tech. **16**, 187 (1981).

[12] V. V. Kveder, Yu. A. Osipian, W. Shcroter, and G. Zoth, Phys. Status Solidi A **72**, 701 (1982).

[13] K. Wuenstel, Solid State Commun. **40**, 797 (1981).

[14] A. Rohatgi *et al.*, Solid State Electron. **23**, 1185 (1980).

[15] G. Zoth and A.G. Siemens (private communication).

[16] J. W. Walker *et al.*, Phys. Rev. **87**, 4587 (1973).

[17] V. V. Kveder *et al.*, Phys. Status Solidi A **87**, 657 (1985).

[18] M. Brohl and H. Alexander, in *Structure and Properties of Dislocations in Semiconductors 1989*, edited by S. G. Roberts *et al.*, IOP Conf. Proc. No. 104 (Institute of Physics and Physical Society, London, 1989), p. 163.

[19] Yu. S. Lelikov, Yu. T. Rebane, S. Ruvimov, A. A. Sitnikova, D. V. Tarhin, and Yu. G. Shreter, Phys. Status Solidi B **172**, 53 (1992).