

Influence of Dislocation Loops on the Near-Infrared Light Emission From Silicon Diodes

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Abstract—The infrared light emission of forward-biased silicon diodes is studied. Through ion implantation and anneal, dislocation loops were created near the diode junction. These loops suppress the light emission at the band-to-band peak around $1.1 \mu\text{m}$. The so-called D1 line at $1.5 \mu\text{m}$ is strongly enhanced by these dislocation loops. We report a full study of photoluminescence and electroluminescence of these diodes. The results lead to new insights for the manufacturing approach of practical infrared light sources in integrated circuits.

Index Terms—Dislocation loops, integrated optics, integrated optoelectronics, light-emitting diodes (LEDs), light sources, luminescent devices, optoelectronic devices, semiconductor device fabrication, semiconductor devices, silicon.

I. INTRODUCTION

INTEGRATED electronics and integrated optics are enabling technologies for the digital age. A breakthrough is expected when electronics and optics can be fully integrated onto a single chip [1]. Currently, light can be transported, split, switched, and detected using integrated components in a microchip. However, a light source that meets all the requirements for full monolithic integration is still being searched. The quest is for an efficient light source operating at (and above) room temperature and preferably emitting in a narrow wavelength range. Red or near-infrared light would be very suitable for communication purposes. The light emitter should be laterally confined and preferably switchable at gigahertz frequencies.

Light-emitting diodes (LEDs) and laser diodes based on III-V semiconductors show excellent technical qualities, but integration of these into a silicon chip has proved far from

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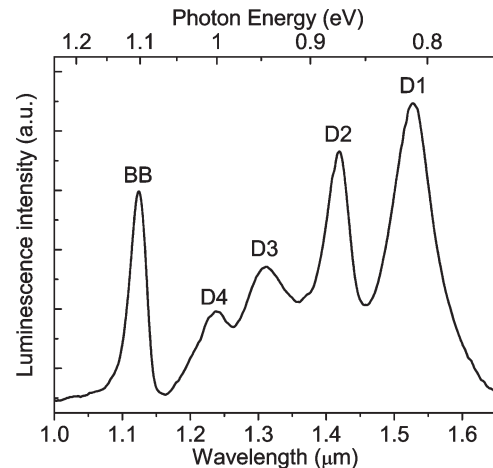


Fig. 1. Typical luminescence spectrum of dislocated Si measured at 80 K. The dislocation-related peaks D1–D4, as well as the BB peak, are indicated in the figure.

straightforward. The use of a silicon diode as LED is complicated by the indirect bandgap. This leads to a long lifetime for radiative recombination and, hence, severe competition from nonradiative recombination processes. Until only a few years ago, the quantum efficiency of a standard silicon diode was assumed limited to 10^{-6} . However, it was recently shown that forward-biased silicon diodes can reach an external quantum efficiency close to 1%, combining standard silicon technology with established techniques from the LED and solar cell industries [2]. The key in reaching high internal quantum efficiency is in the mastering of the competing nonradiative recombination processes: Shockley-Read-Hall (SRH), Auger, and surface recombination [3]. A theoretical maximum efficiency around 20% has recently been predicted for silicon LEDs by several groups [4], [5]. Modern IC technology offers a complete toolkit to make such diodes, and one can further benefit from the high purity of present-day silicon wafers. Silicon also can be prepared to emit at somewhat longer wavelengths, as illustrated in Fig. 1 (after [6]); the D1 peak around $1.5 \mu\text{m}$ is particularly fascinating for the purpose of optical communication.

In various papers, a relation is reported between the quantum efficiency of such silicon LEDs and the presence of dislocation loops [6]–[10]. Dislocation loops can be conveniently formed using ion implantation and subsequent anneal. Therefore, a dislocation-loop-engineered silicon LED emerges as a potential light source for the further integration of electronics and optics. However, the contradicting reports in literature concerning the theoretical explanation of the dislocation loop's role,

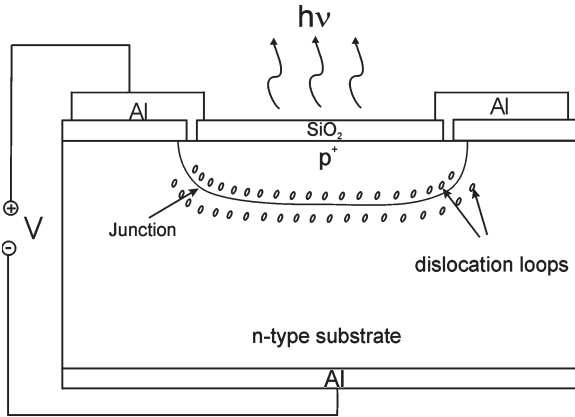


Fig. 2. Cross section of a LED with two dislocation loop arrays formed above and below the p^+/n junction.

as well as contrasting experimental reports, call for further experimentation.

In this paper, we investigated silicon LEDs with deep p^+-n junctions and created dislocation loops around the junction using ion implantation and anneal. In a recent paper [9], we presented evidence that dislocation loops are detrimental to band-to-band (BB) electroluminescence (EL). This paper brings a full account of photoluminescence (PL) and EL in the full wavelength region of interest (1–1.6 μm), which are extended to cryogenic temperatures. Also, further physical analysis using transmission electron microscope (TEM) and high-resolution X-ray diffraction spectroscopy (HRXRD) is presented. A complete and consistent physical picture emerges on the interaction between the dislocation loops and the light emission of silicon LEDs.

II. EXPERIMENTAL DETAILS

A. Device Fabrication

We fabricated p^+n diodes in Cz-grown $5\text{--}10\text{-}\Omega\cdot\text{cm}$ n-type silicon wafers (see Fig. 2). The p^+ region was formed by either 40-keV B^+ ion implantation or by solid-state diffusion from B-doped CVD oxide layers. The B diffusion took place at $950\text{ }^\circ\text{C}$ for 10 min in nitrogen plus 20 min in oxygen. Under this condition, the p^+ sheet resistance and junction depth were in the same range as the B-implanted regions (around $25\ \Omega/\text{square}$ and 400 nm, respectively). The sheet resistance of the p^+ regions was measured with a four-point probe, and the junction depth of the p^+/n junctions was checked with the ball-grooving and staining technique. The dislocation loop formation inside the B-implanted LED was steered by varying the anneal temperature between $850\text{ }^\circ\text{C}$ and $1050\text{ }^\circ\text{C}$, for a fixed time of 20 min.

The diodes formed by B diffusion were optionally implanted with $10^{15}\ \text{Si}^+$ atoms/ cm^2 and subsequently annealed at $950\text{ }^\circ\text{C}$ for 20 min in nitrogen ambient to form dislocation loops. Two implant energies of silicon were used to control the position of the dislocation loops: either above the metallurgical junction, i.e., inside the p^+ region (using 200 keV) or beneath it, i.e., in the n region (with 450 keV). A single B-diffused wafer received all Si implant varieties, by implanting only part of the wafer.

TABLE I
OVERVIEW OF THE SILICON LED PROCESS VARIATIONS. SAMPLES 1–4 ARE ANNEALED AFTER EACH OF THE SILICON IMPLANTS

Nr.	p^+ formation	Si^+ implant ($10^{15}\ \text{cm}^{-2}$)	Anneal
1	diffusion	–	$2 \times 20'$ $950\text{ }^\circ\text{C}$
2	diffusion	200 keV	$2 \times 20'$ $950\text{ }^\circ\text{C}$
3	diffusion	450 keV	$2 \times 20'$ $950\text{ }^\circ\text{C}$
4	diffusion	200&450 keV	$2 \times 20'$ $950\text{ }^\circ\text{C}$
5	40 keV B^+	–	20' $850\text{ }^\circ\text{C}$
6	40 keV B^+	–	20' $900\text{ }^\circ\text{C}$
7	40 keV B^+	–	20' $950\text{ }^\circ\text{C}$
8	40 keV B^+	–	20' $1050\text{ }^\circ\text{C}$

Possible wafer-to-wafer variations (e.g., low-level contamination or thermal budget differences) are thus avoided. (Transient-enhanced boron diffusion caused by the silicon implants [11], [12] will result in slightly different p^+ profiles for each of the diodes. We found no evidence that this affects our results.) Under the given implantation dose, acceleration voltage, and annealing temperature and time, category-II dislocation loops form [13], [14] in two configurations: prismatic dislocation loops and faulted Frank dislocation loops.

Subsequent to the implantation and the final $950\text{ }^\circ\text{C}$ anneal, aluminum was deposited at the front- and backside of the devices, and the front metal patterned. The wafers were then sintered at $400\text{ }^\circ\text{C}$ for 5 min in wet N_2 ambient. The lateral dimensions of the p^+ region (approximately $200 \times 200\ \mu\text{m}^2$) and the test structure geometry of the fabricated LEDs were similar for all those four regions as well as for the case of B-implanted samples. Larger areas were used for the PL measurements.

The details of sample fabrication are summarized in Table I. Variations were made in the formation of the p^+ region, the (optional) lattice-damaging silicon implant, and the thermal anneal. These experiments are intended to verify earlier experimental observations and to improve insight into the mechanisms behind these observations.

B. Measurement Setup

Electrical characteristics were measured using a Cascade probe station and an Agilent 4156C parameter analyzer. The EL was measured under current pulses (1–100 mA) with a frequency of $\sim 30\ \text{Hz}$. The PL from these samples was excited by an Ar-ion laser emitting at 514 nm with an excitation power of 100 mW and a laser-spot diameter of $100\ \mu\text{m}$. The excitation beam was chopped at $\sim 30\text{-Hz}$ frequency. For detection of EL and PL signals, the luminescence was analyzed with a monochromator and a liquid-nitrogen-cooled Ge detector system. A standard lock-in technique was applied to process the luminescence signals.

The LED efficiencies were estimated from the EL BB transition peaks. The spectra were normalized using the spectral response of the system on a calibrated light source. The normalized peaks were then integrated over wavelength. The obtained values were converted to photon flow values at the energy of related peak maxima and divided on the acting value of electron flow to obtain external quantum efficiency. The value for the internal efficiency was estimated by taking into consideration geometrical and reflectivity factors.

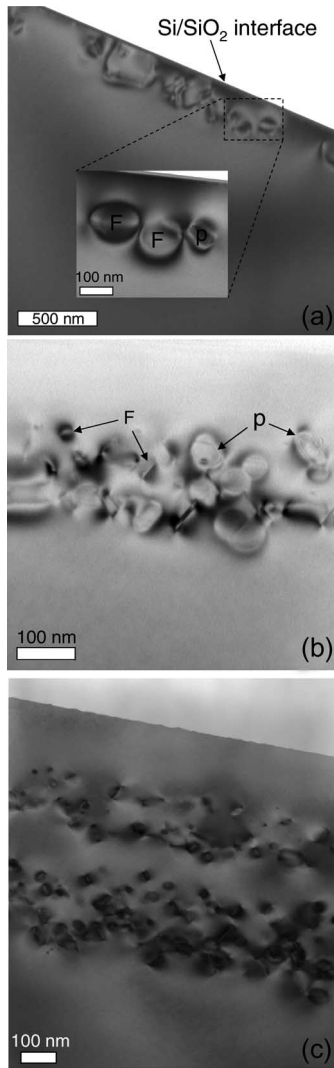


Fig. 3. HRTEM images of dislocation loops on the samples: (a) B-implanted at 40 keV; (b) Si-implanted at 200 keV; and (c) Si-implanted at 200 keV + 450 keV. The prismatic dislocation loops are indicated by the letter p, and the faulted Frank dislocation loops are indicated by the letter F.

III. RESULTS AND DISCUSSION

A. Physical Analysis of the Dislocations

TEM images show that the dominant visible defects in the implanted samples are dislocation loops. In B-implanted samples, the dislocation loops were formed inside a 300-nm region from the sample surface, as shown in Fig. 3(a). In these samples, the implantation creates both the p^+ impurity profile and the lattice damage leading to dislocation loops. Since the dislocation loops form around the peak of the implantation profile (projected range) and always lie before the metallurgical junction, the p/n junction was located beneath the dislocation loops in the silicon substrate for B-implanted samples.

Dislocation loops were observed also in Si-implanted samples, as presented in Fig. 3(b) and (c). Bands of defects are present at depths of 250–350 and 450–670 nm below the Si/SiO₂ interface corresponding to 200- and 450-keV Si implantation, respectively. The density of dislocations is higher than in the B-implanted samples. The diameter of dislocation

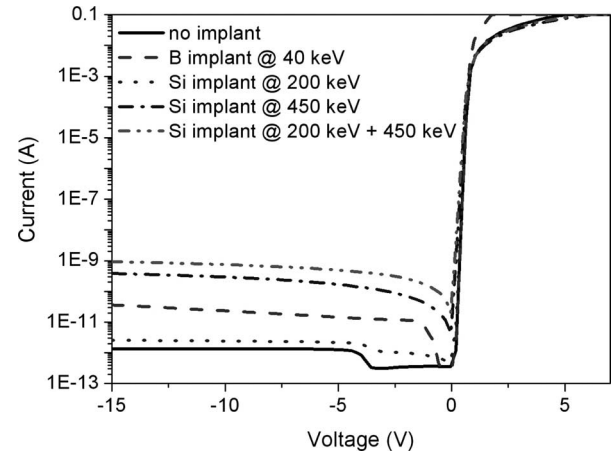


Fig. 4. I - V characteristics of five LEDs: B-diffused without implant; B-implanted at 40 keV; B-diffused with Si implanted at energies of 200, 450, and 200 + 450 keV. All these LEDs were annealed in nitrogen at 950 °C for 20 min.

loops in both Si- and B-implanted samples was in the same ~ 100 -nm range. From the TEM images, it was obtained that the formed defects are mainly prismatic dislocation loops and faulted Frank dislocation loops (indicated in Fig. 3 by the letter p and F, respectively).

By using HRXRD, the crystallographic features of the 200-keV Si-implanted sample were further investigated. As expected, the high boron doping results in tensile strain [15], extending almost 2 μm into the substrate. A compressive strain peak of 0.1 GPa ($da/a = 800$ ppm), which is created by the presence of dislocation loops, is shown at 250–320-nm depth from Si/SiO₂ interface. The TEM and HRXRD results thus confirm that the silicon implantation and subsequent anneal caused dislocation loops in the desired regions.

B. Electrical Properties of the Diodes

Current–voltage (I - V) characteristics were measured at room temperature between the back and front contacts to verify normal diode operation and to investigate the level of generation-recombination currents. The reverse leakage current of the B-diffused diode is very low. This indicates a low contamination level in our devices [16]. All B-implanted diodes also show low leakage currents. In the Si-implanted diodes, the leakage current was larger and increased with dislocation loop density, as shown in Fig. 4. However, the highest reverse-current density at -15 V of a double Si-implanted diode is still at the acceptable level of $2.5 \mu\text{A}/\text{cm}^2$. Under forward bias, the diodes have a swing of 64–72 mV. This good ideality indicates that the recombination process predominantly takes place outside the space charge region throughout the low injection regime.

C. Diode Luminescence at Room Temperature

Infrared light emission is observed in all samples, both under forward biasing (EL) and when excited with an Ar laser (PL). Typical PL and EL spectra are shown in Fig. 5 (taken at cryogenic temperatures in this case). In most cases, the BB

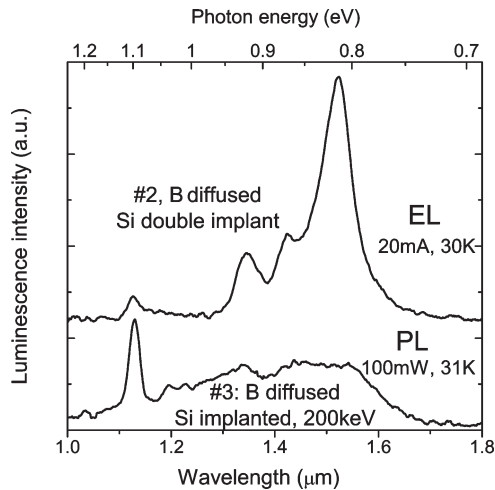


Fig. 5. Typical PL and EL spectra of samples, manufactured with boron diffusion and silicon implantation. The BB and D2–D4 peaks are observed in the spectra. At this low temperature, the D-band EL is dominant, because phonons are required for BB recombination.

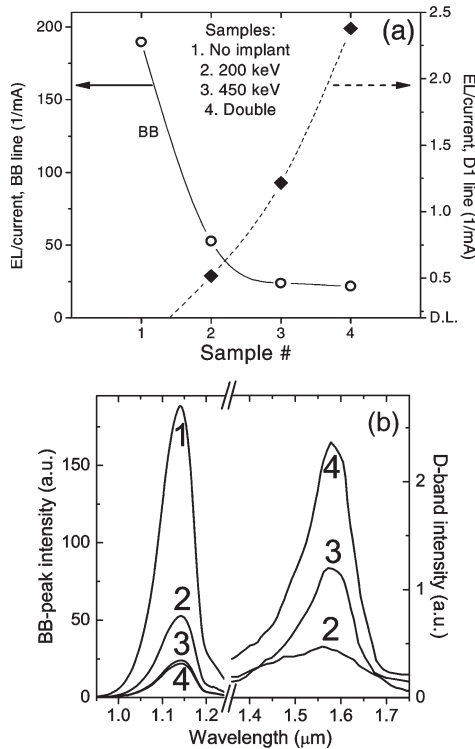


Fig. 6. Results of EL measurements on diodes made with B diffusion, optionally implanted with silicon. (a) The peak intensity of the BB and D1 lines for each of the samples. (b) EL peaks at these wavelengths. Measurements were performed at 300 K, and the diode forward bias was 20 mA.

recombination peak around 1150 nm and the D1 peak around 1500 nm are observed both in the PL and the EL spectra. With our measurements, we have confirmed that the intensity of both emission peaks depends strongly on the presence of silicon lattice damage, presumably the presence of dislocation loops. However, the trend is opposite: More lattice damage leads to an increase in D1 luminescence and a decrease in BB luminescence. This is quantified in Fig. 6. Concerning the BB peak, this result contradicts the assumption by Ng *et al.* [7] that dislocation loops are responsible for enhanced 1.1- μm light

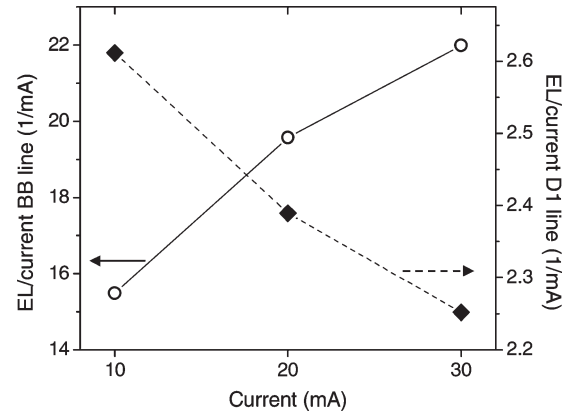


Fig. 7. Dependence of current-normalized EL intensities on the forward current. The data were obtained from a B-diffused double Si-implanted sample (sample 4 in Table I) at 300 K.

emission. This comes on top of earlier arguments [4], [17] that the carrier confinement mechanism proposed in those papers is not likely. Kveder also reported a decrease in BB luminescence in the presence of a high density of dislocation loops [8].

PL measurements confirm a strong BB signal on the B-diffused sample without silicon implantation. The signal from this sample was about 30 times stronger than that from the sample implanted with 200-keV Si^+ ions. In other silicon-implanted samples, at 300 K, the PL signal was below the detection limit.

Although our HRXRD measurements revealed the presence of a high strain field caused by the dislocation loops, no effect of the strain was detected on the BB luminescence peak position and/or shape. This result suggests that most of the BB luminescence originates far away from the loops. Therefore, BB radiative recombination mainly occurs in the defect-free regions of the wafer, as was suggested in [10].

All silicon-implanted samples exhibit D1 luminescence, as well as the B-implanted diode with lowest anneal temperature of 850 °C. Early studies of the lines D1–D4 indicated that the dislocation loops are responsible for the emission [18]. Indeed, we find an increase of D1 emission with increasing lattice damage (caused by silicon implants). Still, by using the implantation-damage approach, the D1 EL remains weak under all conditions. Plastic deformation of silicon, causing much higher dislocation loop densities, in combination with gettering and hydrogen passivation, led to external efficiencies of 0.1%–0.2% [8]—but plastic deformation is difficult to embed into microelectronic fabrication. Efficiency improvement for D1 emission could be feasible by using multiple implantation energies and special implantation geometries.

In Fig. 7, the ELs at the D1 and BB peak are shown in the forward-biased current range from 10 to 30 mA (at much higher injection than reported in [19]). The EL is normalized to current. Superlinear behavior is seen for the BB line, whereas the D1 line has a slight sublinear intensity increase with current. The BB efficiency thus improves at higher injection, whereas the D1 line is attenuating. The observed behavior of BB radiation is consistent with efficiency calculations as a function of the carrier injection level. The BB EL efficiency is expected to decrease at even higher injection levels (when the

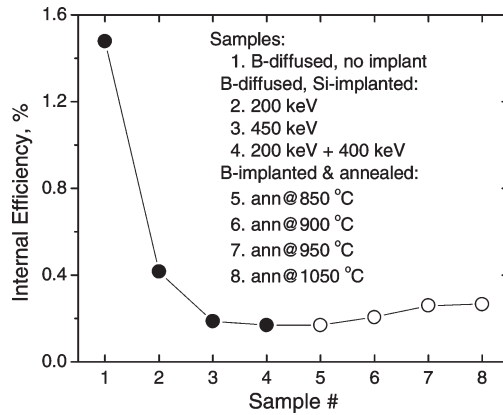


Fig. 8. Internal efficiency of various diodes, estimated from the external intensity of the BB peak at 300 K. Sample numbers are explained in the figure. Results from B-diffused samples are shown with closed circles, and B-implanted samples are shown with open circles.

carrier injection level goes well beyond 10^{17} cm^{-3} , due to a strongly enhanced Auger recombination. For the D1 efficiency versus injection level, the situation is more complex. The SRH mechanism cannot be applied for extended defects [20]. The occupancy of the dislocation states may either gradually saturate at higher injection levels or show a field dependence.

The estimated internal efficiencies of the BB EL at a forward current of 50 mA are shown in Fig. 8 for all diodes. It can be seen that, in the case of B-implanted samples, the presence of dislocation loops leads to a suppression of the BB luminescence. The dislocation loops are formed during annealing, but will dissolve again when annealed at higher annealing temperature. The B-implanted samples annealed at 850 °C are therefore expected to have the highest dislocation loop density [21]. All samples then show that the BB luminescence decreases with increasing dislocation loop concentration.

D. Temperature Dependence of Luminescence

The competitive recombination through dislocation levels and via the BB transition also affects the temperature behavior of the EL. EL spectra recorded at various temperatures from the double-silicon-implanted sample are presented in Fig. 9 (top). As shown in the figure, the low-temperature spectra ($T < 100 \text{ K}$) exhibit a well-pronounced D-band structure, with clearly distinguishable D1, D2, and D3 peaks (compare with Fig. 1). The peaks change shape, intensity, and position as a function of temperature. Data related to the changes in the integrated intensities of the D-band and BB peak and those related to the positions of their maximal intensities are presented in Fig. 9 (bottom).

As shown in Fig. 9, the BB-peak intensity increases substantially starting from $T > 180 \text{ K}$, being under the detection limit at lower temperature. Such an increase in intensity of the BB peak with temperature correlates with that reported previously for P- and B-implanted Si samples [5], [7], [22], and is opposite to the temperature behavior of the BB peak in nonimplanted Si samples [5], [23]. At the same time, a decrease in the integrated intensity of the D-band was observed. Since the intensity of the BB peak in Si-double implanted samples at 300 K is still

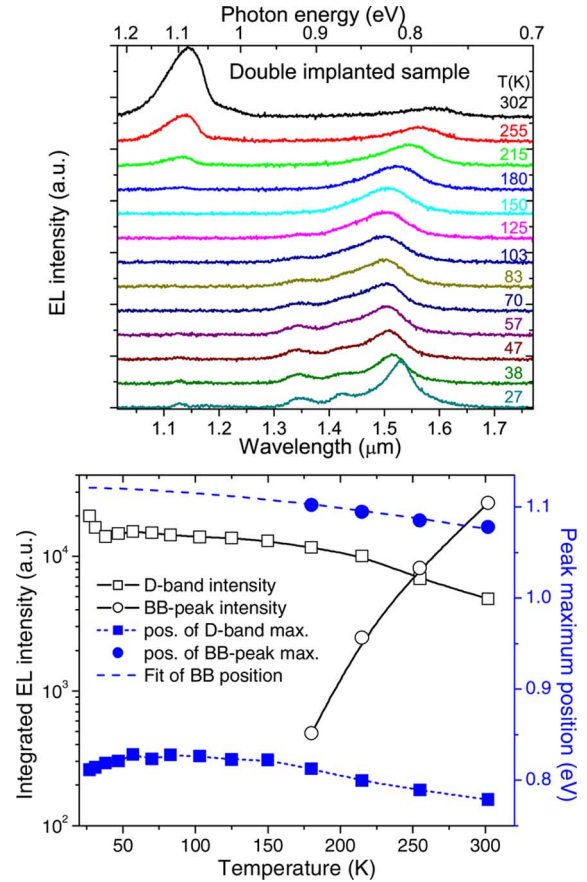


Fig. 9. Top: The EL spectra of a B-diffused double Si-implanted sample at various measurement temperatures. The forward current during the measurements was 20 mA. The curves are shifted in the vertical direction for clarity. In the spectrum detected at 27 K, the D1, D2, and D3 peaks are clearly distinguishable (cf. Fig. 1). Bottom: The signal intensities and positions of maximum intensity, derived from the upper figure. The dashed line shows a fit of the temperature dependence of the BB peak position following the study in [24]. The other lines are drawn to guide the eye.

~ 10 times less than that in nonimplanted ones, we suppose that the anomalous behavior of its intensity is related to redistribution of recombination processes between the BB recombination and the radiative and nonradiative recombination processes related to dislocations. Moreover, comparison of the changing ratios of the signal intensities in Fig. 9 (bottom) leads us to suggest that a substantial part of the dislocation-related recombination processes in the samples are nonradiative. PL from the D-band in the Si-implanted samples was detected at temperatures below 200 K. Similar to EL, the PL intensity of the D-band increased on the order of 200-keV implant \rightarrow 450-keV implant \rightarrow double implant.

The temperature dependence for the position of the maximum intensity of the BB peak corresponds to the expected dependence [24], as illustrated by the fit in Fig. 9 (bottom). The T-dependence for the D-band maximum position is more complex. A similar dependence for the D1 peak, which is reported previously [25], was attributed to the origin of D1 luminescence, i.e., to the radiative transition between two shallow levels related to dislocations.

The emission at $1.1 \mu\text{m}$ is strong at room temperature and above, as earlier reported in [2], [7], [9], and [22].

Room-temperature emission at 1.5 μm is considerably weaker in all our experiments. To determine the best method for the introduction of dislocations into silicon for 1.5- μm LEDs, including plastic deformation [8], wafer direct bonding [10], and ion implantation, further investigations are necessary.

IV. CONCLUSION

The impact of dislocation loops on the infrared light emission from silicon LEDs was studied. Silicon p⁺n diodes were fabricated using boron diffusion, boron and silicon implantation, and thermal anneals. The resulting diodes show a strong variation in the density and physical location of implantation-originated dislocation loops—confirmed by TEM and HRXRD measurements. Strong light emission is observed around the BB recombination wavelength of 1150 nm, which is identified as phonon-assisted radiative recombination. The BB radiation becomes progressively weaker at lower temperature and with increasing dislocation loop density.

D-band luminescence shows the opposite trend, both in temperature and the dislocation loop density. From the found dependences, it is concluded that, with the applied manufacturing techniques (B diffusion, and B and Si implantation), the most efficient room-temperature silicon LED is formed by causing minimum lattice damage, emitting at the BB edge (1150 nm).

Ion-implanted silicon LEDs may present interest for light emission at 1.5 μm ; however, to that purpose, the dislocation loop density must be strongly increased compared to the devices presented here, while nonradiative recombination processes must remain suppressed.

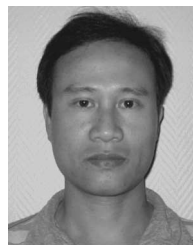
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