Direct bandgap narrowing in Ge LED’s on Si substrates

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Abstract: In this paper we investigate the influence of n-type doping in Ge light emitting diodes on Si substrates on the room temperature emission spectrum. The layer structures are grown with a special low temperature molecular beam epitaxy process resulting in a slight tensile strain of 0.13%. The Ge LED’s show a dominant direct bandgap emission with shrinking bandgap at the $\Gamma$ point in dependence of n-type doping level. The emission shift (38 meV at $10^{20}$ cm$^{-3}$) is mainly assigned to bandgap narrowing at high doping. The electroluminescence intensity increases with doping concentrations up to $3\times10^{19}$ cm$^{-3}$ and decreases sharply at higher doping levels. The integrated direct gap emission intensity increases superlinear with electrical current density. Power exponents vary from about 2 at low doping densities up to 3.6 at $10^{20}$ cm$^{-3}$ doping density.

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OCIS codes: (130.3120) Integrated optics devices; (230.3670) Light-emitting diodes; (160.3380) Laser materials.

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Received 28 Nov 2012; accepted 9 Jan 2013; published 22 Jan 2013
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#180727 - $15.00 USD
1. Introduction

Light sources are an important requirement for future photonic applications in Si photonic integrated circuits. Efficient light sources from a Si based heterostructure will gain importance in the growing field of Si based photonics [1, 2]. However the realization of integrated light emitters with Si, SiGe and Ge are still challenging because of the indirect band structure. Recent Ge based laser work proved that an indirect semiconductor with a direct transition not far above the indirect one (136 meV in case of Ge) could be a light source with high integration potential on Si [3, 4]. A direct semiconductor could be obtained by high tensile strain (1.8%) in Ge [5] or by the incorporation of the larger atom Sn in the Ge lattice. It is predicted that Ge_{1-Z}Sn_Z alloys turn into direct group IV semiconductor crystals if Z amounts to more than 10% [6]. In the last years different groups already demonstrated room temperature direct band gap electroluminescence (EL) from indirect semiconductor Ge [7–11] on Si. Tensile strain from thermal expansion mismatch (typically 0.15% to 0.25%) and high n-doping increase the luminescence emission efficiency.

In highly doped semiconductors the bandgap shrinks with increasing doping level because of the effect of bandgap narrowing. Band gap narrowing in heavily doped semiconductors is caused by ionized impurity potentials, by impurity band formation and many electrons interaction. In electronic devices it is described by an apparent increase in intrinsic carrier concentration [12]. In Si the bandgap narrows by 90 meV at 10^{20} cm^{-3} doping. In Ge different values are assigned for the indirect L minimum and the direct Γ gap narrowing [13]. The direct gap narrowing varies between 30 meV and 70 meV (extrapolated) at doping levels from 10^{19} cm^{-3} to 6x10^{19} cm^{-3}. The L minimum (indirect transitions) shows a slightly larger narrowing (by 15 meV to 30 meV) compared to the direct narrowing [13, 14]. In Ref [14], the indirect L minimum narrowing is dependent on the doping type described as slightly larger for p-doping than n-doping (95 meV vs. 80 meV at 6x10^{19} cm^{-3}). The effect of bandgap narrowing is observed with photoluminescence (PL) measurements at Ge LED’s [15]. In this paper we investigate the influence of n-type doping (doping concentration between 5x10^{17} cm^{-3} and 1x10^{20} cm^{-3}) of the direct band gap EL of Ge LED’s.

2. Epitaxial growth and device fabrication

The Ge heterojunction p’nn’ LED’s are fabricated in a quasi-planar technology with a heterostructure top contact [16]. The technology is based on a sequential growth of layers by solid source molecular beam epitaxy (MBE) [17]. The MBE machine is equipped with a Si electron beam evaporator and a special Ge effusion cell. As n and p dopant sources, Sb and B effusion cells are used. The layer sequence and the annealing steps are grown with one epitaxial run. The schematic cross section of the layer stack is shown in Fig. 1(a). B-doped Si (100) substrates with a high specific resistance ρ > 1000 Ωcm are used.

The growth starts with the buried layer (BL) contact which is very high B doped of about 10^{20} cm^{-3}. This BL contact consist of a 100 nm thick virtual substrate (VS) and a 300 nm p’ Ge layer. The VS accomplishes the accommodation of the lattice constant of Ge (4.2% larger than Si) to the underlying Si by a dense network of misfit dislocations at the Si interface. The
technical realization of the VS is performed by low temperature growth of 50 nm Ge (330 °C) followed by a high temperature annealing step (810 °C). A second 50 nm thick p’ doped Ge layer grown at 330 °C smooth the annealed surface and a further temperature annealing step at 750 °C completes the VS. The 300 nm p’ Ge layer completes the layer growth of the buried layer (BL) contact. A third annealing step at 750 °C adjusts the tensile strain in the BL material. This is an important step for the following growth steps, because Sb-doped Ge cannot be annealed at temperatures higher than 500 °C. The surface segregation of Sb in Ge is very strong depending on growth temperature [18]. To achieve an abrupt transition of Sb-doping the growth temperature is decreased in a growth interruption to 160 °C. In a growth series the doping concentration nvar of the 300 nm thick n-Ge layer are varied between 5x10^{17} cm^{-3} and 1x10^{20} cm^{-3}. In addition a reference pin LED is grown. The n’-doped top contact is finally realized as a highly Sb-doped (10^{20} cm^{-3}) Ge/Si heterojunction contact [16]. The device processing by mesa etching, passivation and metallization is the same as with earlier reported vertical Ge pin photodiodes [16, 17]. The complete realized LED is shown in a plan view scanning electron microscopy image in Fig. 1(b).

The tensile strain (caused by the larger thermal expansion coefficient of Ge compared to the Si substrate) of the LED’s is engineered by a high temperature annealing step at the end of the BL growth. A tensile strain increases the lattice constant of Ge and shifts the bandgap slightly more into the infrared [19]. In a following growth step the Ge layers are grown with the same lattice parameters as the underlying BL. The determination of the strain status of the LED’s is possible with EL peak position measurements at a reference pin LED grown with the same procedure [19]. In principal, the Sb doping could decrease the tensile strain in the n-Ge layer because the Sb atom has got a higher covalent radius (0.138 nm) as the Ge atom (0.122 nm). However the concentration of Sb in Ge is smaller than 0.2% and its influence (below 0.03%) can be neglected for the strain analyses of the p’nn’ Ge LED’s.

3. Electrical and optical characterization

The room temperature current density -voltage (J-V) characteristics are measured with a Keithley 4200 semiconductor parameter analyzer. Figure 2(a) displays the corresponding J-V characteristics of p’nn’ Ge LED’s with different doping concentrations nvar. The current increases dramatically with increasing doping concentration nvar because of additional tunneling current parts (Zener tunneling, Esaki tunneling).

The J-V characteristics of the Ge LED with different device areas (doping concentration nvar = 3x10^{19} cm^{-3}) are presented in Fig. 2(b). In the forward characteristics the current scales with the device area up to 0.4 V. For higher voltages (> 0.4 V) the J-V characteristics does not scale with the device area because the series resistance of the devices is limiting the current. In the reverse characteristics the Zener tunneling current scales with device area up to 0.1 V. At higher voltages the influence of the series resistance is seen, too. The inset in Fig.
2(b) shows the linear plot of the J-V curve of the smallest device with a radius of 1 µm. A negative differential resistance (NDR) is found with a peak to valley current ratio (PVCR) of 1.07. A diode with this I-U characteristic is called Esaki diode. An NDR is a strong indicator for abrupt junctions and excellent layer quality [20]. The challenges for the Esaki structures are the abrupt doping transitions and the defect levels in the epi layers which should be low in order to avoid high excess currents.

Fig. 2. (a) J-V characteristics of p⁺n⁻ Ge LED’s with different doping concentrations n_var in the n-Ge layer. (b) J-V characteristics of a p⁺n⁻ Ge LED with different device areas at a constant doping concentration of n_var = 3x10¹⁹ cm⁻³. The inset shows the linear plot of the J-V curve with a negative differential resistance.

For light emission the p⁺n⁻ Ge LED is operated in forward direction at high current densities where the impact of series resistance is strong. In order to minimize the series resistance it is beneficial to use a layout with both contacts on the upper side of the wafer to circumvent the high resistance of the substrate.

Fig. 3. (a) Direct gap room temperature EL spectra of 80 µm radius Ge p⁺n⁻ LED’s under different injection current densities. Active n-type region is 3x10¹⁹ cm⁻³ (left) and 4x10¹⁹ cm⁻³ (right) doped. (b) Integral EL intensity of a 80 µm radius p⁺n⁻ Ge LED’s as function of doping concentration at different current densities.

The setup for the EL measurements consists of a semiconductor parameter analyzer, a probe station with a glass fiber and an Ando AQ6315A optical spectrum analyzer (OSA). A multimode glass fiber with 800 µm core radius is adjusted above the emitting surface of the Ge heterojunction pin LED to collect the light and is directly connected to the OSA. The range of the OSA goes from 350 nm to 1750 nm, but low signals are difficult to detect at > 1700 nm due to increasing noise of the internal InGaAs detector. Figure 3(a) shows the typical room temperature EL spectra I_EL as function of energy of p⁺n⁻ Ge LED’s at different forward injection current densities. The active n-type region is n_var = 3x10¹⁹ cm⁻³ (left) and n_var = 4x10¹⁹ cm⁻³ (right) doped. This small difference in the doping concentration changes the emission of more of a factor of 2.3. The EL measurements are analyzed in two steps, the
integral gap EL versus injected current and the EL peak position as function of electrical power.

The integral direct gap EL intensity $P^{\Gamma}$ is calculated with:

$$P^{\Gamma} = \int I_{EL}(E)dE$$  \hspace{1cm} (1)

The result of $P^{\Gamma}$ versus doping concentration of the complete growth series is shown in Fig. 3(b). The intensity increases with increasing of the n-type doping up to $3 \times 10^{19}$ cm$^{-3}$. For higher doping concentration an abrupt decrease of the emission is found. We found for all doping concentrations a superlinear relation $P^{\Gamma} \sim j^m$ with the power exponent $m$. This implies that the LED is more efficient when operated under high injected current. An example for the dependence of $P^{\Gamma}$ versus $j$ at a doping concentration of $n_{var} = 3 \times 10^{19}$ cm$^{-3}$ is shown in the inset in Fig. 4. The extracted exponent $m$ is here 2.25. The complete overview of the exponents $m$ of all samples is shown in Fig. 4. The exponent $m$ is in the range of 2 between $5 \times 10^{17}$ cm$^{-3}$ and $3 \times 10^{19}$ cm$^{-3}$. At higher doping concentration $n_{var}$ the exponent increases up to 3.61 for $1 \times 10^{20}$ cm$^{-3}$.

![Graph showing the relation between Exponent m and Doping concentration n var](image)

Fig. 4. Exponent m versus doping concentration $n_{var}$ of the $P^{\Gamma} \sim j^m$ characteristics of the investigated LED’s. Inset: Integrated emission to current density characteristics of a 80 µm radius p+nn+ Ge LED with a doping concentration of $n_{var} = 3 \times 10^{19}$ cm$^{-3}$. The exponent $m$ is 2.25.

The EL spectra exhibit a band to band optical transition with peaks around the direct bandgap energy. The energy of the EL peak shifts with increasing injection current because the high injection currents increase the device temperature by heating. Nevertheless, temperature can be deduced from the shape of the spectrum. The emission intensity $I_{EL}(E)$ is composed of the contributions of the 3D density of states which constrains the low energy emission and of the approximated Boltzmann-distribution for the high energy tail:

$$I_{EL}(E) \sim \sqrt{E - E_g} \cdot \exp\left(-\frac{E}{k_B T}\right)$$  \hspace{1cm} (2)

where $E$ is the photon energy, $E_g$ the direct bandgap energy, $k_B$ the Boltzmann constant and $T$ the absolute temperature. Therefore the EL maximum $E_{max}$ is located at a photon energy of:

$$E_{max} = E_g + \frac{k_B T}{2}$$  \hspace{1cm} (3)

Accordingly curve fitting of the emission spectra leads to an independent identification of the parameters $E_g$ and $T$. The inset in Fig. 5 shows the direct bandgap energy as function of...
electrical power for the p'nn' Ge LED with $n_{\text{var}} = 3 \times 10^{19} \, \text{cm}^{-3}$. A clear linear dependence is found. The intersection with the energy axis i.e. the extrapolation to zero electrical power leads to the direct bandgap energy at room temperature. For this Ge LED a value of 0.759 eV is calculated.

The bandgap energy as function of doping concentration $n_{\text{var}}$ is plotted in Fig. 5. The bandgap shrinks with increasing of the Sb doping level. This effect is caused by the bandgap narrowing in heavily doped semiconductors. Figure 5 shows also the bandgap of the pin Ge reference LED (blue hexagon). The sole difference between the reference pin and the p'nn' Ge LED is the doping of the n zone. The intrinsic region has got a background doping of p-type with a doping concentration of $10^{16} \, \text{cm}^{-3}$. For the pin Ge LED a direct $\Gamma$ gap of 0.79 eV is calculated from the EL measurements. This means that the direct bandgap shifts in the infrared about 10 meV compared with unstrained Ge. A shift of 10 meV corresponds with a tensile strain of 0.13% [21]. The growth strategy particularly with regard to growth temperature profile of all samples is the same. This means that all samples have got roughly a tensile strain of 0.13% and the direct bandgap in all samples is decreased by 10 meV compared with unstrained, low doped Ge. The bandgap of n-doped Ge as calculated from peak emission energies (equ. 2) follows in a semilog plot (Fig. 5) a linear relation above a threshold of about $10^{18} \, \text{cm}^{-3}$. The slope (red line in Fig. 5) is weaker than expected from published absorption curves [13, 14, 22]. The peak emission shifts 38 meV to lower energy at a doping level of $10^{20} \, \text{cm}^{-3}$.

4. Conclusion

In conclusion, we analyzed the direct bandgap EL from tensile strained Ge heterojunction p'nn' LED’s on Si substrates as function of doping concentration. The layer structure is grown with MBE with a special heterostructure top contact. The NDR in the LED with a doping concentration of $3 \times 10^{19} \, \text{cm}^{-3}$ shows the excellent layer quality. A maximum room temperature emission at a LED with a radius of 80 µm is found at a doping level of $n_{\text{var}} = 3 \times 10^{19} \, \text{cm}^{-3}$. For higher doping concentrations an abrupt decrease of the emission is seen. We found for all doping concentrations a superlinear relation between the optical power and the injected current. For doping concentrations larger than $n_{\text{var}} = 3 \times 10^{19} \, \text{cm}^{-3}$ the exponent $m$ increase up to 3.61 for $1 \times 10^{20} \, \text{cm}^{-3}$. The tensile strained Ge LED’s shows a shrinking of direct bandgap in dependence of the Sb doping concentration with a maximal shift of 38 meV at $n_{\text{var}} = 1 \times 10^{20} \, \text{cm}^{-3}$. This effect is caused by the bandgap narrowing in heavily doped semiconductors but the slope is smaller than expected from published absorption curves in highly n-doped Ge.