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RESEARCH ARTICLE

Direct band gap luminescence from Ge on Si pin diodes

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Abstract Germanium (Ge) pin photodiodes show clear direct band gap emission at room temperature, as grown on bulk silicon in both photoluminescence (PL) and electroluminescence (EL). PL stems from the top contact layer with highly doped Ge because of strong absorption of visible laser light excitation (532 nm). EL stems from the recombination of injected carriers in the undoped intrinsic layer. The difference in peak positions for PL (0.73 eV) and EL (0.80 eV) is explained by band gap narrowing from high doping in n^+-top layer. A superlinear increase of EL with current density is explained by a rising ratio of direct/indirect electron densities when quasi Fermi energy level rises into the conduction band. An analytical model for the direct/indirect electron density ratio is given using simplifying assumptions.

Keywords photoluminescence (PL), electroluminescence (EL), germanium (Ge), direct band gap

1 Introduction

Direct gap photoluminescence (PL) in germanium (Ge) was measured at low temperature (2 K) as early as 1978 [1]. But only recently PL and electroluminescence (EL) [2,3], optical gain [4] and optical pumped lasing [5] were demonstrated from Ge on silicon (Si). Efficient light sources from a Si based heterostructure will gain importance in the growing field of Si based photonics [6,7]. Direct band gap EL was explained to be promoted by tensile strain [2] or high doping [3]. The energy position of the PL and EL was claimed as indication of the same optical transition mechanism for optical and electrical excitation [2,3]. The PL was however not monitored from the full device structure [2], but from a reference layer without electrical contact layer. We investigated PL and EL from the full device structure, which had an optical window in the top metallization. Furthermore, the doping in the contact layers was chosen that high ($10^{20}/cm^3$) that band gap narrowing should allow an unambiguous discrimination of band gaps in intrinsic and doped regions.

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2 Growth and device processing

The growth of the complete layer stack by molecular beam epitaxy (MBE) on a high resistivity ($>1000\,\Omega\cdot$cm) p-Si substrate, the device processing by mesa etching, and the passivation and metallization are the same as with earlier reported vertical Ge pin photodiodes [8–11]. A cross section of the structure below the top window is given in Fig. 1. A virtual substrate (VS) accomplishes the accommodation of the lattice constant of Ge (4.2% larger than Si) to the underlying Si substrate by a dense network of misfit dislocations at the Si interface. Technical realization of the VS is performed by low temperature growth of Ge (330°C) followed by two high temperature annealing steps (850°C,

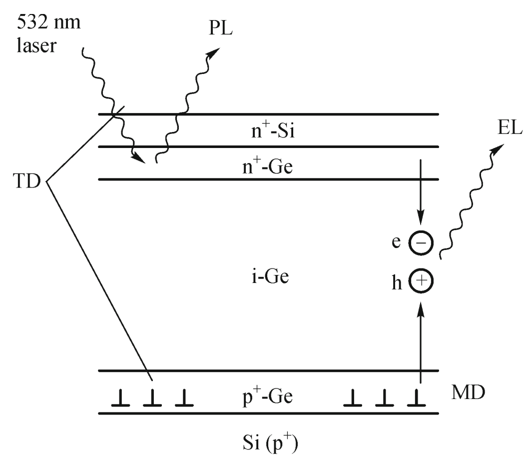

Fig. 1 Basic scheme of Ge pin structure and of luminescence experiments. MD misfit dislocation network; TD threading dislocation; photoluminescence (PL) with 532 nm laser excitation; electroluminescence (EL) via recombination of injected electrons (e) and holes (h)

620°C). For the sake of easier integration with Si-microelectronics, this VS is chosen very thin (100 nm). As trade off, we accept a higher density of threading dislocation (TD) (in the 10^7/cm^2 to 10^8/cm^2 range) as with thicker graded SiGe buffer layers. The VS is p$^+$-doped (B, 10^{20}/cm^3) and serves as buried ground contact for the EL experiments. A 500 nm intrinsic (i) Ge-layer follows which is grown at low temperature (330°C) to suppress segregation of doping. After 700°C anneal, a very low temperature (160°C) n$^+$ (Sb, 10^{20}/cm^3)-top contact layer finishes the epitaxy. Abrupt doping profiles and full activation of dopants are confirmed by secondary ion mass spectrometry (SIMS) and electrical resistivity measurements [12,13].

3 Luminescence measurements

PL measurements are performed with laser light of 532 nm wavelength [14] and cw-power levels of 100 mW to 1 W. The penetration depths in Si and Ge are 4 μm and 15 nm, respectively.

The excitation light is therefore absorbed in the top n$^+$-Ge contact layer. Only a small fraction of the photo-generated carriers will reach the intrinsic Ge-layer below because the diffusion length in highly doped material is limited by the Auger recombination. The measured room temperature PL-spectrum shows in Fig. 2. The dominating peak is at about 0.73 eV with a broad shoulder on the low energy side. The peak below 0.5 eV is assumed to be the main dislocation line. A clear but weaker peak is seen on the higher energy side at about 0.8 eV which is the direct band gap in intrinsic Ge.

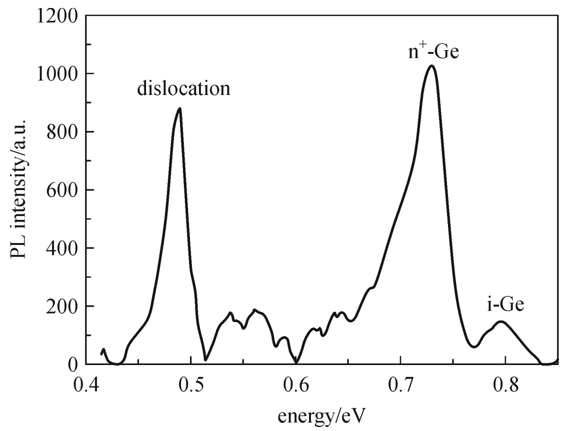

Fig. 2 PL spectrum of the Ge-pin photodiode (mesa diameter: 160 μm). Main lines are assigned (from left) to dislocations, narrowed direct band gap luminescence from n$^+$ top layer (0.73 eV), and direct band gap luminescence from intrinsic Ge (0.80 eV)

EL can be observed by application of a forward bias on the pin structure. The electrons and holes injected into the intrinsic Ge-layer recombine there, partly emitting light in competition with radiationless recombination processes. The main features of the EL-spectrum should correspond to the intrinsic Ge layer. Indeed, the major line (Fig. 3) is around 0.8 eV (direct gap of i-Ge) with satellites in the 0.7 eV region. No strong line is visible in the indirect band gap energy region (0.664 eV- phonon energy). The intensity of the 0.8 eV peak is super linear depending on current density (EL ~ $I^{1.7}$). With lower ambient temperature, the intensity of the EL peak decreases strongly (to about 1/20 at 80 K).

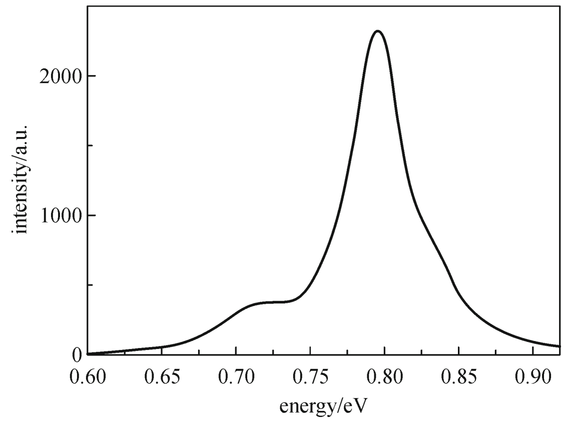

Fig. 3 EL spectrum of Ge-pin photodiode. Forward biased to 200 mA; Main line (0.80 eV) is from the direct gap of intrinsic Ge

Main tasks for explanations of the experimental facts are the dominance of the direct transition in an indirect semiconductor and the distinct different peak positions of the PL and EL characteristics, respectively. As we will now show that the difference in the peak position is caused by the band gap narrowing in heavily doped semiconductors.

4 Band gap narrowing in doped semiconductors

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 [15] by an apparent increase in intrinsic carrier concentration. In Si, the band gap 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 [16]. The direct gap narrowing varies between 30 and 70 meV (extrapolated) at doping levels from 10^{19}/cm^3 to 6×10^{19}/cm^3. The L minimum (indirect transitions) shows a slightly larger narrowing (by 15 to 30 meV) compared to the direct narrowing [16,17]. In Ref. [17], the indirect L minimum narrowing is given as dependant on the doping type described as slightly larger for p-doping than n-doping (95 meV versus 80 meV at 6×10^{19}/cm^3).

In our PL experiment, the exciting laser light (532 nm) is absorbed mainly in the n$^+$-Ge cap layer (Fig. 1). The peak position in luminescence of a doped semiconductor has to reflect the redshift from band gap narrowing and the blueshift (Burstein shift [18]) from Fermi energy level rise above the corresponding band edge. The occupied states below the Fermi energy level cause a blueshift as the maximum of carriers shifts from near band edge at low doping to the Fermi energy at higher doping. This effect is very pronounced in direct semiconductors, where the Fermi level rise in the conduction band above effective density of states levels (typically 10^{18} range). In indirect semiconductors, only the weak indirect emission is strongly influenced by this effect, the higher lying direct band is less influenced, in n^+-Ge the Fermi level touch the direct band at around 10^{20} doping. Indeed the main PL-peak (Fig. 2) is at 0.73 eV that is the 70 meV narrowed direct transition from the n-doped top layer (in undoped, unstrained Ge the direct transition is expected at 0.80 eV). A much smaller peak appears at 0.80 eV that stems from photo-exited carriers diffusing into the intrinsic Ge layer below. Unexplained in this article is the low energy shoulder at around 0.7 eV, which could be related to dislocation levels [14]. At the position of the indirect gap (0.664 meV at room temperature), only weak indications of optical transitions and their phonon replica are visible.

5 EL energy

The EL [19] signal is mainly generated in the intrinsic Ge region (Fig. 1) by the recombination of carriers injected from both highly doped sides. The main peak (Fig. 3) at 0.8 eV reflects the direct transition in i-Ge. The satellites at around 0.70–0.74 eV could be caused by carriers penetrating into the opposite doped region. From PL, we know the contribution from the n^+-side, the p^+-side could broaden the signal shoulder because of slight position differences for p-type narrowing. As in PL, no distinct indication of indirect transitions (phonon replica in EL to be expected around 0.65 eV) could be identified.

The dominance of the direct radiative transitions in the indirect semiconductor Ge is caused by: (1) much faster direct recombination, (2) low energy difference (136 meV) between direct (0.80 eV) and indirect transition (0.664 eV), (3) quasi-Fermi energy level shifted between direct and indirect conduction band edge by high electron levels. Let us assume an equilibrium of carriers within the separated bands (valence, conduction band), which allows to describe the carrier statistics by quasi-Fermi energy levels. The faster direct recombination yields a dominant direct peak, even if the occupation of the direct valley is much smaller than the indirect one. At rather low carrier injection, the Boltzmann approximation is valid for the occupation statistics of both, direct and indirect states. The ratio of direct to indirect states n_d/n_{ind} is then constant and expressed by a proportionality with $\exp(-\Delta E_C/kT)$. At room temperature, this exponential term in Ge is about 0.4%. For higher injection, this ratio increases when the quasi Fermi level rises above the conduction band edge.

6 Trends of occupation statistics with high carrier injection

We give a simplified model based on equal effective masses for the conduction subbands and a quasi-Fermi level position within the indirect band calculated with $T = 0$ K. Both assumptions allow to analyze clearly the general trend but the numerical values depend on the choice of effective masses. The electron density should be high enough that the quasi-Fermi energy E_{Fn} is above the indirect L minimum E_{Cind} but below the direct gap E_{Cd} (Fig. 4). This would be fulfilled with electron densities from $3\times10^{18}/cm^3$ to $10^{20}/cm^3$. From basic semiconductor theory [20], one can find the densities n_d, n_{ind} of direct (Γ) electrons and indirect (L) electrons, respectively.

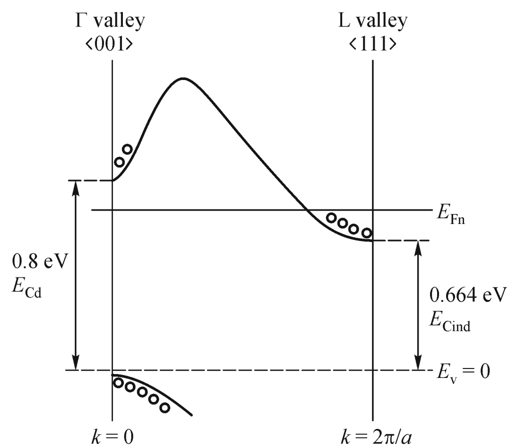

Fig. 4 Occupation scheme of the Ge conduction band with direct gap (Γ). The Fermi energy E_{Fn} is assumed to be above the L valley (see text)

Boltzmann-approximation (valid for $E_{Cd} - E_{Fn} > 0$)

$$n_d = N_C \exp\left(-\frac{E_{Cd} - E_{Fn}}{kT}\right), \tag{1}$$

($T = 0$ K approximation for $E_{Cind} - E_{Fn} < 0$)

$$n_{ind} = \frac{2}{3} Const \cdot (E_{Fn} - E_{Cind})^{3/2}. \tag{2}$$

The constant *Const* and the effective density of states N_C are dependent on the effective mass m^* (density of states effective mass)

$$N_C = 2\left(\frac{2\pi m^* kT}{h^2}\right)^{3/2}, \tag{3}$$

$$Const = 8\sqrt{2}\pi \frac{m^{*3/2}}{h^3}. \tag{4}$$

Replacement of E_{Fn} in Eq. (1) by using Eq. (2) delivers the relation between direct n_{d} and indirect n_{ind} densities.

$$\ln n_{\mathrm{d}} = -\Delta E_{\mathrm{C}}/kT + \ln N_{\mathrm{C}} + (3\sqrt{\pi}/4)^{2/3}(n_{\mathrm{ind}}/N_{\mathrm{C}})^{2/3}. \quad (5)$$

The third term in Eq. (5) describes the nonlinear increase of n_{d} with respect to n_{ind} when the quasi-Fermi level is between the both band edges (indirect, direct). The nonlinear relation between n_{d} and n_{ind} is given by

$$\ln\left(\frac{n_{\mathrm{d}}}{n_{\mathrm{ind}}}\right) = -\frac{\Delta E_{\mathrm{C}}}{kT} + \left(\frac{3}{4}\sqrt{\pi}\right)^{2/3}\left(\frac{n_{\mathrm{ind}}}{N_{\mathrm{C}}}\right)^{2/3} - \ln\left(\frac{n_{\mathrm{ind}}}{N_{\mathrm{C}}}\right). \quad (6)$$

Note, the validity of this approximation is restricted to

$$1 < \frac{n_{\mathrm{ind}}}{N_{\mathrm{C}}} < \frac{4}{3\sqrt{\pi}}\left(\frac{\Delta E_{\mathrm{C}}}{kT}\right)^{3/2}, \quad (7)$$

according to the assumed Fermi energy.

The first term in Eq. (6) gives the relation for the Boltzmann approximation ($n_{\mathrm{ind}} < N_{\mathrm{C}}$), the second and third term describe the increase in relative occupation between direct and indirect states when the Fermi level enters the conduction band. The second and third term deliver always a positive amount that means an increase of the ratio between direct and indirect densities as shown in Table 1. This is a consequence of the Fermi-Dirac statistics which then cannot be approximated by simple exponential terms (Boltzmann approximation). The ratio increase of direct states compared to indirect one is probably responsible for the nonlinear current density dependence of EL.

Table 1 Density ratio of direct /indirect states ($\ln(n_{\mathrm{d}}/n_{\mathrm{ind}})$) given as function of the normalized carrier density $n_{\mathrm{ind}}/N_{\mathrm{C}}$. The model (Eq. (6)) is assumed with ΔE_{C} = 136 meV and T = 300 K

$\frac{n_{\mathrm{ind}}}{N_{\mathrm{C}}}$	Boltzmann	1	3	10
$\ln\left(\frac{n_{\mathrm{d}}}{n_{\mathrm{ind}}}\right)$	−5.5	−4.3	−4.1	−2.2

7 Conclusions

Dominant direct band gap emission from Ge pin photodiode on Si could be confirmed for PL and EL. Based on band gap narrowing argument, the main contribution could be assigned to emission from the top n^{+}-layer in PL and to emission from the intrinsic layer in EL. An analytical occupation model for the ratio of electrons in direct Γ minima and indirect L minima is in agreement with the observed nonlinear current dependence of EL. Fermi-Dirac statistics delivers an increasing ratio of direct states to indirect states, if the Fermi level rises into the conduction band above the band edge but below the direct transitions.

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