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Room Temperature Direct Band Gap Electroluminescence from Ge-on-Si Light Emitting Diodes

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We report the first demonstration of direct band gap electroluminescence (EL) from Ge/Si heterojunction light emission diodes (LEDs) at room temperature. In-plane biaxial tensile strain is used to engineer the band structure of Ge to enhance the direct gap luminescence efficiency by increasing the injected electron population in the direct $\Gamma$ valley. Room temperature EL is observed at the direct gap energy from a Ge/Si p-i-n diode exhibiting the same characteristics of the direct gap photoluminescence (PL) of Ge. The integral direct gap EL intensity increases superlinearly with electrical current due to an indirect valley filling effect. These results indicate a promising future of tensile strained Ge-on-Si for electrically pumped, monolithically integrated light emitters on Si.

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Recently, there has been a surge in research on Si-based light emitters for Si optoelectronic applications owing to the potential for monolithically integrating optical components with electronic devices on Si. Electronic-photonic integration on Si meets the needs for high-bandwidth and low-power-density on-chip interconnects [1,2]. Since Si shows a very inefficient band-to-band radiative recombination due to its indirect band gap nature, erbium-doped silicon dielectrics [3-6] and silicon Raman effect [7,8] have been used for light emission at the desired wavelength band around 1550 nm. However, the challenge of electrical pumping for the above approaches remains to be solved. Electrical injection can be realized in hybrid integration solutions with a III-V laser either bonded to a silicon waveguide [9] or grown on relaxed, graded GeSi buffer layers [10]. However, a monolithic integration approach is more appealing owing to far less expensive fabrication cost that enables high volume manufacturing. Germanium as the active material is a promising candidate for monolithically integrated Si-based light emitters because of its high compatibility with silicon complimentary metal oxide semiconductor (CMOS) processes and its 1550nm (0.8 eV) light emission from direct band-to-band transition [11]. In this letter, we demonstrated the first Ge light emitting diode (LED) exhibiting direct gap emission in the wavelength range of 1535 to 1660 nm at room temperature.

Unlike silicon, germanium has a direct band gap only slightly larger than its indirect band gap by 0.136 eV. This pseudo direct band gap structure allows a small portion of electrons to be injected into the direct conduction band minimum (Γ valley) under pumping and radiatively recombine with holes in the valence band with very little loss from nonradiative processes due to the high optical transition rate of direct band-to-band transition. This direct gap photoluminescence has been demonstrated in thin crystalline germanium films either polished from bulk Ge [12] or bonded as a top layer in Ge-on-insulators [13]. However, the overall light
emission efficiency is low, because the majority of the injected electrons stays in the indirect band minima (4-fold degenerate L valleys) according to Fermi distribution, and the indirect transition rate is 4-5 orders of magnitude lower than the direct transition so that most of the electrons recombine nonradiatively [14]. To increase the injected electron population in the Γ valley so as to increase the overall light emission efficiency, in-plane tensile stress is introduced into epitaxial (100) Ge thin films on Si. The thermally induced tensile strain shrinks the direct band gap relative to the indirect band gap, resulting in more injected electrons in the direct Γ valley following Fermi statistics. According to previous theoretical calculations, Ge would become a direct band gap material at 2% tensile strain [15]. However, such high strain is not favorable since it is difficult to achieve and it will shrink the band gap to 0.5 eV (2500 nm) which is far away from the desired wavelength range for optical interconnects (near 1550 nm). Instead, we introduce 0.2%-0.25% tensile strain in Ge films aiming at the proper wavelength range as well as achieving good materials quality [16,17]. The remaining energy difference between the direct and indirect band gaps can potentially be compensated by n-type doping to fill the indirect L valleys with extrinsic electrons so that more injected electrons stay in direct Γ valley as discussed in our previous work [11]. As an initial step towards the final goal, we have fabricated tensile strained Ge/Si p-i-n diodes to investigate the direct gap electroluminescence (EL) of Ge.

The cross-section of the p-i-n heterojunction diode is schematically shown in Fig. 1(a). A hot-wall ultra-high vacuum chemical vapor deposition (UHVCVD) reactor was used to selectively grow epitaxial Ge on boron-doped p⁺ Si (100) substrates with a resistivity of 0.005 Ω cm. A SiO₂ layer deposited on the silicon substrate was patterned to expose certain regions of Si for the Ge selective growth [18]. A 50 nm Ge buffer layer was first grown at 335°C to kinetically
suppress island formation. A 1.7 μm thick Ge layer with a root-mean-square surface roughness less than 1 nm was then grown at an elevated temperature of 700 °C. Details about this two-step growth method were reported in Ref [19]. Post-growth thermal annealing at 900 °C was performed to reduce the threading dislocation density to $1.7 \times 10^7$ cm$^2$ measured from etch pit density studies. The Ge film was fully relaxed at the annealing temperature, and tensile strain was introduced by cooling to room temperature due to the large thermal expansion coefficient difference between Ge and Si [20]. As a result, an in-plane tensile strain of 0.2% was introduced into the Ge film, causing a reduction of the direct band gap between the minimum of the $\Gamma$ valley and the maximum of light-hole band to 0.76 eV [17].

A poly Si film was then deposited on top of the Ge film and implanted with $\sim 10^{20}$ cm$^{-3}$ phosphorus to form the n-type electrode for the p-i-n heterojunction diode. Aluminum was used as the electrical contact material and individual diode was insulated by SiO$_2$. An example of the microscopic image of the fabricated device is shown in Fig. 1(b).

The I-V characteristics of the fabricated tensile strained Ge/Si heterojunction diodes were measured by a HP-4145A semiconductor parameter analyzer. The I-V curve shown in Fig. 1(c) is measured from a 20 μm by 100 μm rectangle-shaped diode and exhibits a good rectifying behavior with a dark current of $5 \times 10^{-5}$ A at 1 V reverse bias. In EL measurements we forward biased the diode from 0.5 to 5.5 V for carrier injection.

The EL characteristics of the Ge diodes were measured by an Ando AQ6315E optical spectrum analyzer. A multi-mode fiber was placed above the device to collect the light emission from the surface. The optical spectrum analyzer was connected to the other end of the fiber to detect the emission spectra. We observed the onset of EL from the 20 μm by 100 μm diode at a forward bias of 0.5 V, corresponding to an injection current of 1.3 mA. Fig. 2(a) shows the EL
spectrum at room temperature from the diode at 50 mA forward electrical current. The spectrum exhibits a band-to-band optical transition that peaks around the direct band gap energy of 0.77 eV. The full width at half maximum (FWHM) is about 60 meV, in good agreement with the ~2 kT peak width of direct gap transitions. The spectrum is also consistent with the room temperature photoluminescence (PL) measured from a 0.2% tensile-strained epitaxial germanium film on silicon [21] shown in Fig. 2(b). A 488 nm Ar ion laser was used in the PL measurement and the spectral response was measured by a Hamamatsu R5509-72 photomultiplier tube (PMT) through a grating monochromator. The steeper drop of the intensity in the PL spectrum than in the EL spectrum near 0.75 eV is due to the dramatic decline in responsivity of the PMT. The small red shift in the EL peak position compared to PL peak position is due to the heating effect under the injection current that slightly reduces the band gap. To our knowledge, this is the first observation of direct gap EL from any Ge devices. The characteristics of the EL and of the PL are in a great agreement indicating the same direct gap optical transition mechanism for both electrical injection and high energy photon (488 nm, 2.5 eV) optical injection. The multiple sharp peaks in the EL spectrum are reproducible and not due to noise. The linear relationship between the energy positions of these peaks and the peak number shown in the Fig. 2(a) inset indicates the occurrence of Fabry-Perot resonances corresponding to an air gap of ~120 µm between the end of the optical fiber and the device surface.

The integral direct gap EL intensity shows a superlinear relationship versus the injected electrical current, as shown in Fig. 3. This phenomenon is described by the following formula:

$$\text{EL}_{\text{dir}} \propto n_e(\Gamma) = n_e(\text{total}) f(\Gamma)$$

(1)

The integral direct gap EL intensity is proportional to the electron concentration in the direct Γ valley \( n_e(\Gamma) \) which depends on both the total injected electron concentration \( n_e(\text{total}) \) and a
fraction term, $f(\Gamma)$, reflecting the percentage of the electrons in the $\Gamma$ valley. The first term scales linearly with the injected electrical current, while the second term also increases with the injection level due to the increase of the quasi Fermi level resulting in more electrons scattered into the direct $\Gamma$ valley. The multiplication of these two terms results in a superlinear behavior of the integral EL with electrical current. The theoretical calculation based on this model is shown by the solid curve in Fig. 3 and it agrees well with the experimental data. The small difference between the theoretical and the experimental result is possibly due to the small deviation from the square-root density of states near the band edge. This result also supports the theory that the direct gap luminescence benefits from an indirect valleys filling effect by either carrier injection or n-type doping [12].

In conclusion, we demonstrate the first direct band gap EL from a Ge LED on Si at room temperature. Tensile strain is introduced into Ge to enhance the direct gap luminescence efficiency by shrinking its direct band gap relative to its indirect band gap therefore increasing the electron population in the direct $\Gamma$ valley. The room temperature direct gap EL spectrum is consistent with the PL spectrum we reported earlier. The integral EL intensity increases superlinearly with electrical current because the direct gap luminescence efficiency benefits from an indirect valley filling effect to scatter more electrons to the direct valley under injection, which agrees with our theoretical calculation. These results show the potential of tensile strained Ge-on-Si as a promising candidate for electrically pumped, efficient monolithic light emitters on Si.

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Fig. 1: (a) Schematic cross-section of a tensile-strained Ge/Si heterostructure p-i-n light emitting diode. (b) The microscopic image of the top view of a 20 μm by 100 μm Ge/Si p-i-n diode. (c) The I-V characteristics of the Ge diode.

Fig. 2: (a) Direct gap electroluminescence spectrum of a 20 μm by 100 μm 0.2% tensile-strained Ge/Si p-i-n light emitting diode measured at room temperature. The multiple sharp peaks in the spectrum are highly periodic. The linear behavior of the peak position versus peak number, shown in the inset, demonstrates a periodicity of 5.3 meV due to Fabry-Perot resonances between the device surface and the end of the coupling fiber. (b) Room temperature direct gap photoluminescence of a 0.2% tensile-strained Ge film epitaxially grown on silicon.

Fig. 3: Integral electroluminescence intensity of a 20 μm by 100 μm 0.2% tensile-strained Ge/Si p-i-n light emitting diode increases superlinearly with electrical current due to an indirect valley filling effect. The theoretical calculation (solid line) agrees well with the experimental result.
Fig. 1
Fig. 2

(a) EL (a.u.)

(b) PL (a.u.)

Photon Energy (eV)
Fig. 3