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Direct gap photoluminescence of n-type tensile-strained Ge-on-Si

Xiaochen Sun, a) Jifeng Liu, Lionel C. Kimerling, and Jurgen Michel
Microphotonics Center, Massachusetts Institute of Technology, Bldg. 13-4118, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139, USA

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Room temperature direct gap photoluminescence (PL) was observed from n-type tensile-strained epitaxial Ge-on-Si. The PL intensity increases with n-type doping due to a higher electron population in the direct Γ valley as a result of increased Fermi level. The direct gap emission also increases with temperature due to thermal excitation of electrons into the direct Γ valley, exhibiting robustness to heating effects. These unique properties of direct gap emission in an indirect gap material agree with our theoretical model and make Ge a promising light emitting material in 1550 nm communication band. © 2009 American Institute of Physics. [DOI: 10.1063/1.3170870]

The realization of silicon photonics requires a Si-based light emitter capable of integration with electronic integrated circuits. Compared to hybrid solutions involving III-V lasers either bonded to Si waveguides1 or grown on relaxed graded GeSi buffer layers,2 a complimentary metal oxide semiconductor compatible integration is more desirable for high volume manufacturing Ge has been proposed as a very promising candidate to make such a light emitter.3 Ge is a Si-compatible material and a potentially efficient light emitter at its direct gap energy 0.8 eV (1550 nm) due to its pseudo-direct gap nature. Our previous theoretical calculations suggested that tensile strain and n-type doping can be applied to enhance the direct gap light emission of Ge.4 In this letter, we demonstrate significant enhancement in room temperature direct gap photoluminescence (PL) of tensile-strained epitaxial Ge-on-Si by n-type doping. The temperature-dependent direct gap PL measurement is also discussed to show the unique property of direct gap emission in an indirect gap material predicted by our model.

Ge is normally recognized as a poor light emitting material due to its indirect band structure. The radiative recombination through indirect transition is inefficient as a result of a phonon-assisted process. Therefore, indirect gap PL was only observed from high-purity single crystalline bulk Ge at cryogenic temperatures.5 The direct transition in Ge, on the other hand, is a very fast process with radiative recombination rate of four and five orders of magnitude higher than that of the indirect transition,5 so that the direct gap light emission of Ge is as efficient as that of direct gap III-V materials. The challenge is to have a sufficient number of electrons in the direct Γ valley of the conduction band because most of the electrons are pumped into the lower energy indirect L valleys (fourfold degenerate) following the Fermi distribution. Fortunately, Ge is a pseudodirect bandgap material because of the small energy difference (0.136 eV) between its direct gap and its indirect gap. Klingenstein et al.6 observed this direct gap emission at low temperature by using high power density excitation lasers.7 To reduce the excitation level, a better way is to dope Ge with n-type impurities to have L valleys filled with extrinsic electrons. Due to this indirect valley states filling effect and subsequent increase in Fermi level, at the same excitation level the injected electron density in the Γ valley of n+ Ge is significantly higher than in intrinsic Ge, resulting in a stronger direct gap light emission.

Compared to bulk Ge, epitaxial Ge thin films can be further engineered for more efficient direct gap light emission. We can introduce in-plane biaxial tensile stress in epitaxial Ge using the thermal expansion mismatch between Ge and Si.8–10 The induced tensile strain shrinks the direct bandgap relative to the indirect bandgap.3 This effect makes Ge more direct bandgap such as enabling more electrons to be injected into the direct Γ valley at the same excitation and doping level.

The Ge films were epitaxially on Si (100) substrate by using a hot-wall ultrahigh vacuum chemical vapor deposition (CVD) reactor. PH3 was used during growth to incorporate n-type donor phosphorus with concentrations ranging from 1017 to 1019 cm−3. A 60 nm Ge buffer layer was directly grown on Si at a 360 °C to kinetically suppress island formation. A 1 μm thick Ge layer was then grown at an elevated temperature of 650 °C. Postgrowth rapid thermal annealing at 780 °C for 30 s was performed to reduce threading dislocations and to activate the dopants. Details about this two-step growth method were reported earlier.11 The Ge film was fully relaxed at the annealing temperature, and tensile strain was accumulated upon cooling to room temperature due to the large thermal expansion coefficient difference between Ge and Si.8–10 The thermally induced tensile strain in Ge films was measured to be 0.22% by x-ray diffraction (XRD) analysis of (400) and (422) peaks. The thermally induced tensile strain is independent of the phosphorous doping level since it has little effect on the thermal expansion coefficient of Ge.12 A deformation potential modified k·p calculation showed that the direct bandgaps from the minimum of the Γ valley to the maximum of the light-hole band and the heavy-hole band are 0.76 and 0.78 eV, respectively, at this strain level.9,13 A 1 μm thick SiO2 capping layer was deposited by plasma enhanced CVD before postgrowth thermal annealing to prevent out-diffusion of phosphorus. The SiO2 layer was then removed before the PL studies on the Ge films.

A 515 nm Ar ion laser was used in the PL studies. The excitation power density used in the experiment ranges from 0.6 to 60 W/cm². A liquid-nitrogen-cooled InGaAs photodetector and a grating monochromator were used to measure PL spectrum. The spectral response of the PL system ranges

a)Electronic mail: sunxc@mit.edu.
from 800 nm (1.55 eV) to 1770 nm (0.70 eV), well covering the entire direct gap emission wavelength range of 0.22% tensile-strained Ge. The active doping concentrations of the samples were measured by Hall effect at room temperature.

The PL spectrum shown in Fig. 1 is measured from an epitaxial Ge film with $1 \times 10^{19}$ cm$^{-3}$ active $n$-type doping. The PL peak located at about 0.78 eV (1590 nm) corresponds to the direct optical transition at the direct bandgap energy of tensile-strained Ge. The full width at half maximum (FWHM) of the peak is 52 meV, which is slightly larger than the theoretical FWHM of 45 meV for a single band-to-band transition because the strain-induced valence band splitting leads to two closely spaced transitions. Calculated PL spectra of optical transitions from the $\Gamma$ valley to the heavy-hole band and to the light-hole band are shown in Fig. 1. The overlap of the two PL spectra from these two transitions causes the broadening of the overall peak. The PL intensity from the $\Gamma$ valley to the light-hole band is weaker than that to the heavy-hole band due to a lower joint density of states. The experimental PL extends a little more into longer wavelengths compared to what was predicted by band-to-band transition model, indicating the deviation from ideal square root joint density of states. This deviation is a unique property of the direct gap PL from indirect valence states fill- ing effect. High $n$-type doping fills the energy states in the indirect $L$ valleys and increase the Fermi level, which results in a higher injected electron population in the $\Gamma$ valley under excitation. All PL spectra were measured at room temperature. All spectra exhibit the same shape and peak position underlying the phosphorous has negligible effect on either the direct bandgap or tensile strain in Ge. Doping-induced bandgap narrowing (BGN) effect has negligible influence on the direct bandgap since it mainly affects the conduction band minima (for $n$-type doping), which are the indirect $L$ valleys in Ge. A plot of the enhancement of integral PL intensity with active doping concentration is shown in Fig. 2(b). The calculated PL intensity versus doping is are shown with solid line in Fig. 2(b), exhibiting good agreement with the experimental data.

A temperature dependence study of PL was performed on a Ge film with 0.22% tensile strained and $1 \times 10^{19}$ cm$^{-3}$ $n$-type doping. Figure 3(a) shows a series of PL spectra at temperatures from 220 to 300 K. Contrary to the indirect gap PL in Ge or direct gap PL in III-V materials such as GaAs, the direct gap PL of Ge increases with temperature. This unusual phenomenon is due to the fact that the direct $\Gamma$ valley is not the minimum of the conduction band in Ge. As a result, increase in temperature allows an increasing number of electrons, contributing to enhanced direct gap emission, to be thermally excited from the lower energy indirect $L$ valleys to the higher energy direct $\Gamma$ valley following the Fermi distribution. The exponential increase in electron population in the direct $\Gamma$ valley with temperature dominates the effect of nonradiative recombinations in this case since the radiative recombination lifetime of the direct gap transition is much faster than the nonradiative recombination for the epitaxial Ge film. This increase in PL intensity with temperature is a unique property of the direct gap PL from indirect
bandgap materials such as Ge. The above analysis also explains why the direct gap PL in Ge could hardly be observed below 200 K, because very few injected electrons exist in the direct \Gamma valley. Since the increase in the direct gap PL with temperature is a thermally activated process as explained above, an Arrhenius relation of the integral PL intensity with temperature is expected and is confirmed by the experimental data in Fig. 3(b). An activation energy of 1.01 ± 0.003 eV was derived from linear regression fitting. This activation energy is exactly equal to the calculated energy barrier of 0.102 eV between the valence band to the valence band.

A linear relation of the PL peak position with temperature shown in the Fig. 3(a) inset represents the temperature dependence of the direct bandgap of Ge. The temperature coefficient of \( \frac{dE_{\text{d}}}{dT} = -2.2 \times 10^{-4} \text{ eV/K} \) derived from linear regression fitting is less than that of the direct bandgap for bulk Ge (\(-4 \times 10^{-4} \text{ eV/K}\)) in this temperature range. This difference is a result of the increase in thermally induced tensile strain in Ge upon cooling, which reduces the bandgap to partially compensate the temperature-induced bandgap increase.

In conclusion, room temperature direct gap PL from n-type tensile-strained epitaxial Ge-on-Si films was observed and investigated. The direct gap PL peak is located at 0.78 eV (1590 nm) corresponding to the direct band-to-band optical transition from the direct \Gamma valley to the valence band. The increase in PL intensity with either n-type doping or temperature exhibits unique properties of direct gap PL from an indirect bandgap material. The integral PL intensity increases with n-type doping concentration because of an indirect valley states filling effect leading to an increased injected electron density in the direct \Gamma valley that contributes to the direct gap PL. The direct gap emission also increases with temperature due to the thermal excitation of electrons from the indirect L valleys into the direct \Gamma valley following the Fermi distribution. The experimental results agree very well with our model. These findings indicate that Ge is a promising light emitting material in 1550 nm wavelength band.

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