Opto-Electronic Applications of Si/Si$_{1-x}$Ge$_x$ Heterostructures

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Photoluminescence and electroluminescence can be observed in Si$_{1-x}$Ge$_x$/Si heterostructures grown by Rapid Thermal Chemical Vapor Deposition (RTCVD) from 2K to 300K and with peak wavelengths from 1.2 to 1.5 μm. This paper describes the emission mechanisms and a model for their temperature dependence.

Introduction

Despite the enormous progress in the field of silicon VLSI in the past 30 years, practical light emitting devices on silicon substrates have remained an elusive goal. To overcome the problem of indirect bandgap, it has been proposed that certain short-period Si$_{1-x}$Ge$_x$ superlattices would have a direct bandgap due to zone folding effects [1]. It is also known, however, that in a random semiconductor alloy with an indirect bandgap, electrons and holes may recombine directly without phonons to emit light [2]. This is because the randomness of the alloy breaks the perfect translational symmetry of the crystal, and hence relaxes the requirement for momentum conservation. In photoluminescence spectra, this leads to a "no-phonon" (NP) line in addition to the usual phonon replicas in indirect bandgap semiconductors. This effect has been observed in relaxed bulk Si$_{1-x}$Ge$_x$ layers [3], single strained Si$_{1-x}$Ge$_x$ films [4], and in strained Si$_{1-x}$Ge$_x$ quantum wells and superlattices [5]. This paper describes photo- and electroluminescence results based on this alloy randomness effect in strained Si$_{1-x}$Ge$_x$/Si quantum well structures.

Experiments and Modelling

The samples in this work were grown by Rapid Thermal Chemical Vapor Deposition (RTCVD), which is described in more detail in Ref. 6. The samples consist of single or multiple quantum wells of strained Si$_{1-x}$Ge$_x$, followed by Si capping layers. The Si layers were grown from dichlorosilane in hydrogen at 700°C, and the Si$_{1-x}$Ge$_x$ layers were grown at 625°C by adding germane to the above gases. Typical photoluminescence spectra at 2K are described in Refs. 5 and 7. To summarize, the PL is due to excitons bound by impurities at 2K and consists of the no-phonon line near the bandgap, a weak transverse acoustic replica ~15 meV below the NP line, and a series of transverse optical (TO) phonon replicas, the largest of which is the Si-Si mode ~58 meV below the NP line. At temperatures above 10K, the bound excitons become free excitons (or an electron hole-plasma at high pump powers [8]), but little change in the PL spectra is seen (except for broadening due to thermal and electron-hole plasma effects). Typically the luminescence intensity changes by less than a factor of two from 2K to 77K in structures grown by RTCVD. That the mobile free excitons do not all recombine non-radiatively at midgap defects confirms the high quality of the CVD-grown layers.

Above 77K, a strong decrease in the luminescence intensity is observed (Fig. 1 and 2 for x=0.2, x=0.35, respectively). The temperature above which the luminescence decays strongly depends on the germanium factor x in the well. For example, for x=0.2, the NP luminescence intensity has dropped by a factor of ten at a temperature of 160°C, while for x=0.35 this is not observed until 270°C. Furthermore, the activation energies for the decay of the two signals are 180 and 270 meV, respectively, close to the expected bandgap offsets with respect to silicon.
This implies that a large bandgap offset from the cladding Si is necessary for high temperature luminescence. Modelling shows that despite the large drop in PL intensity at high temperatures, nearly all carriers are still confined to the Si₁₋ₓGeₓ layer, however. To explain the decreased luminescence, it becomes necessary to assume a much lower recombination lifetime in the Si cladding layers than in the Si₁₋ₓGeₓ alloy, so that recombination in the silicon controls the overall recombination even though most carriers are in SiGe. This could be explained by defects at the substrate interface or recombination at the top silicon surface. With such a model, the PL intensity (I) can be expected to scale as

$$I \propto T^{-3} \left(1 + C \frac{W_{Si}}{W_{SiGe}} \ e^{-\Delta E/kT} \right)^{-1}$$  (1)

where $W_{Si}$ and $W_{SiGe}$ are the widths of the Si and SiGe active regions and where C is a constant representing the ratio of effective SiGe to Si lifetimes. Using a single value of C, good agreement between the model and data is achieved (Fig. 2).

The luminescence can be pumped electrically by placing the Si₁₋ₓGeₓ quantum wells in the i-region of a p-i-n diode. At 4K, the NP and TO features in this sample are clearly evident by PL and at the energy expected for the composition (Fig. 3), indicating recombination from band-edge carriers and not from defects. Similar features, although thermally broadened, are seen by PL at 77K. In electroluminescence experiments at a heat sink temperature of 80K, the spectra are broader still due to a higher junction temperature, but the similarity to the 77K PL shows that the same band-edge mechanism is responsible for the light. At a heat sink temperature of 300K, emission is still observable with a peak from the NP signal at 1.34 µm (Fig. 4). At room temperature, the EL intensity increased linearly above a threshold density of 250 A/cm², with an estimated lower limit to the internal quantum efficiency of 0.03% [9].

To investigate longer wavelength emission, a 1 nm Ge layer was grown at 625°C followed by a silicon cap. At room temperature, structure electroluminescences over a broad range with a peak at 1.5 µm (Fig. 5). However, at temperature, neither the PL or EL is well defined, so that one cannot identify the luminescence mechanism. It is possible that the light emitted in this structure originates from defects or band-edge carriers. Indeed, if no mixing occurred, one could not expect the NP mechanism to be present in pure Ge layers.

The temperature dependence of the peak intensity of the $x=0.35$ LED of Fig’s. 3 and 4 is shown in Fig. 6, along with the model results of the photoluminescence of Fig. 2. One sees that the EL decay is much slower than the PL decay for the same composition. Also shown is EL intensity vs. temperature for the $x=0.2$ LED’s of Robbins et al. [10]. While the $x=0.2$ LED decays at a much lower temperature than that of the $x=0.35$ LED, it also decays much slower than the PL for similar composition. The reason for the relatively slow decay of the EL at high temperature is presently under investigation.

Summary

The decay of the luminescence at high temperatures in strained Si₁₋ₓGeₓ/Si heterostructures appears to be controlled by recombination outside of the Si₁₋ₓGeₓ layers, so that room temperature photo- and electro-luminescence requires a sufficiently large bandgap offset and a low density of non-radiative centers. Using a Si₀.₆₅Ge₀.₃₅ quantum well grown by RTCVD, an LED with peak emission of 1.3 µm and room temperature quantum efficiency of 0.03% has been achieved. The support of NSF, ONR, and the NJ Commission on Science and Technology is gratefully acknowledged.

Fig. 1. Photoluminescence for various temperatures for Si/strained Si$_{1-x}$Ge$_x$/Si single quantum wells with (a) $x=0.2$ and (b) $x=0.35$.

Fig. 2. Peak no-phonon (NP) PL intensity vs. temperature and model for the data of Fig. 1.

Fig. 3. 4K and 77K photoluminescence and 80K (heat sink) electroluminescence (I=10 mA) for ten Si$_{0.65}$Ge$_{0.35}$ quantum wells in a p-i-n diode.

Fig. 4. 300K (heat sink) electroluminescence (I=15 mA) for the diode of Fig. 3.

Fig. 5. 4K and 77K photoluminescence and 77K and 300K (heat sink) electroluminescence (I=90 mA) of a single 1-nm Ge layer with a Si cap.

Fig. 6. Temperature dependence of electroluminescence for $x=0.2$ (Ref. 10) and the $x=0.35$ LED of Fig's. 3 and 4.