Island Scaling Effects on Photoluminescence of Strained SiGe/Si (100)

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ABSTRACT

The fabrication of electronic devices on semiconductor islands is becoming increasingly common because of silicon-on-insulator technology and/or because of strain engineering in compliant substrate approaches. While photoluminescence can be an accurate probe of Ge content and strain, in islands it can be affected by the presence of the island edges. Here we present data and a model showing that for high quality SiGe, edge effects are critical for sizes under ~20 μm. These effects can be mitigated by regrowing epitaxial silicon to passivate the recombination states on the island edges.

INTRODUCTION

A recent trend in advanced transistor technologies is the fabrication of devices on semiconductor islands or mesas. Silicon-on-insulator (SOI) technology is increasingly popular because of its lower voltage/power and higher speed capabilities compared to traditional bulk Si. When combined with trench isolation between devices, SOI often yields silicon islands. High mobility channel techniques also often utilize islands. For example, strain engineering on compliant substrates [1], crystal-orientation engineering [2], and some novel device structures [3] all require the use of islands.

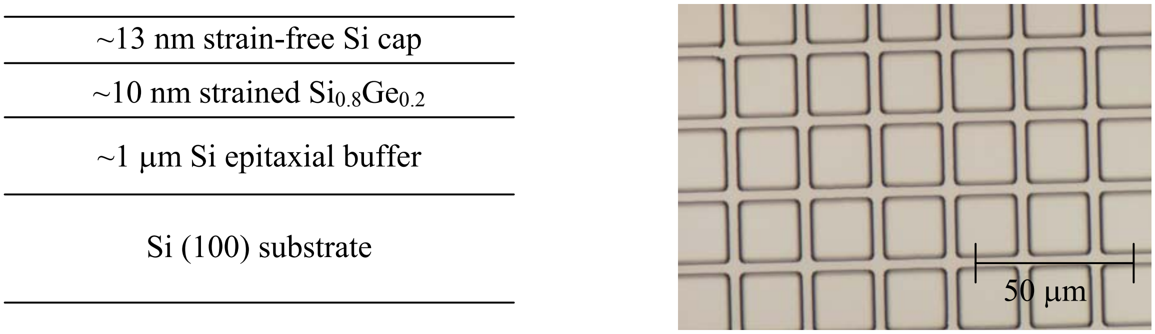
Photoluminescence (PL) is a useful and non-destructive means of characterizing epitaxial layer strain and quality as well as alloy content. When used on island structures, however, the island edges may affect the photoluminescence spectrum. This work experimentally investigates these island edge effects, proposes a model to explain and fit the results, and demonstrates a way to partially mitigate the edge effects.

EXPERIMENT

Silicon (Si) and silicon-germanium (SiGe) epitaxial layers were grown by rapid-thermal chemical vapor deposition. Using an HF-last process, an n-type silicon (100) substrate is wet-cleaned and then cleaned *in situ* with a high-temperature, high-pressure (250 Torr) bake in hydrogen ambient. A ~1 μm silicon buffer layer is grown at a pressure of 6 Torr with 3 lpm (liters per minute) hydrogen carrier flow and 4.33×10^{-7} m^3s^{-1} dichlorosilane, at a temperature of approximately 1000^oC.

The growth continues with a pseudomorphic ~10 nm $Si_{0.8}Ge_{0.2}$ layer, capped with a ~13 nm silicon layer, as shown in figure 1(a). The compressively strained SiGe layer is grown at 625^oC using dichlorosilane and 0.8% germane in hydrogen, and the strain-free silicon cap is grown at 700^oC using dichlorosilane in hydrogen. Further growth details can be found in reference 4.

Square island arrays are dry-etched using SF_6 and O_2. The island edge lengths measure from 5 to 500 μm with inter-island spacings of 1 to 20 μm, respectively. An array of 20 μm islands is



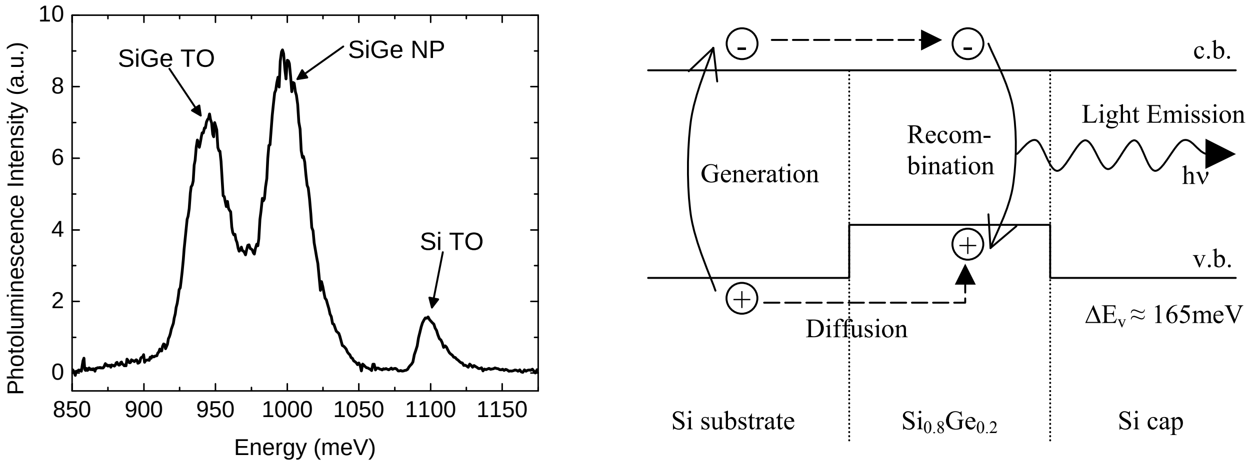
(a) (b)

Figure 1. (a) Epitaxial layer cross-section (not to scale) and (b) Optical micrograph of an array of 20 µm islands.

shown in figure 1(b). Photoluminescence is measured using a 514 nm Argon ion laser at 77K with typical pump power of 0.8W and spot size of 2mm.

RESULTS

The photoluminescence spectrum of an unpatterned sample is shown in figure 2(a). Band-edge PL in SiGe/Si structures comes from the recombination of carriers (or excitons) in the SiGe layer. The carriers are generated in substrate silicon. Holes diffuse to be collected by the SiGe, as shown in figure 2(b), and then electrically attract electrons [5]. PL for silicon results from carriers that recombine in the silicon substrate before making it to SiGe. PL from the $Si_{0.8}Ge_{0.2}$ layer consists of two peaks, one from recombination assisted by transverse optical (TO) phonons (~945 meV) and one from non-phonon (NP) recombination, which occurs due to alloy scattering (~1000 meV). Only the TO peak is observed from the silicon substrate (~1100 meV). In unpatterned samples, most carriers recombine in SiGe so that SiGe PL peak intensities are about five times that from the silicon substrate. No dislocation or defect peaks are visible, indicating coherent growth and good epitaxial interface quality [5].



(a) (b)

Figure 2. (a) Photoluminescence of 13 nm Si / 10 nm $Si_{0.8}Ge_{0.2}$ / Si, measured at 514 nm and 77K and (b) Energy band diagram of the Si-SiGe-Si stack and schematic of generation, carrier transport and recombination processes.

Effect of island pattern

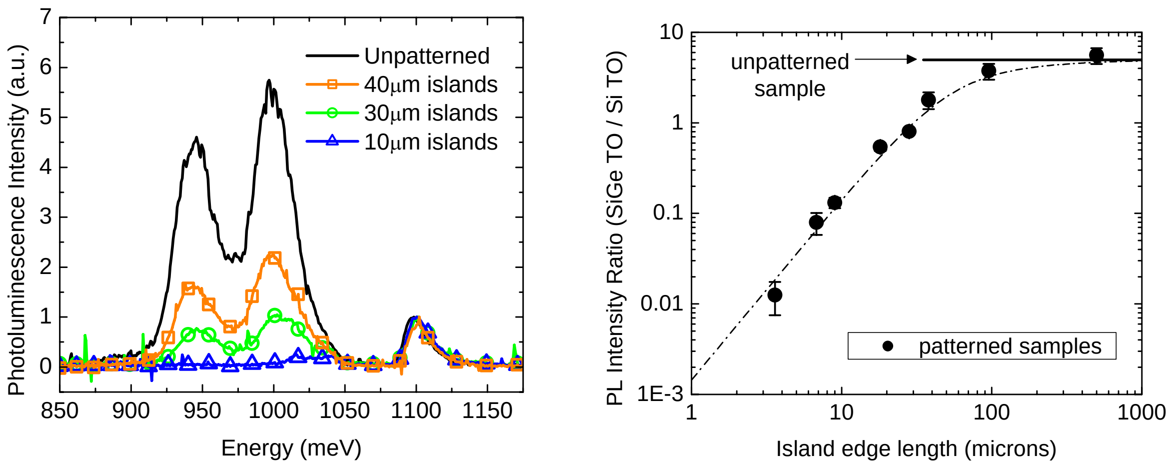
In figure 3(a), photoluminescence of unpatterned and patterned samples are plotted for comparison. For island sizes less than 100 µm, the SiGe TO (and NP) peak heights, relative to the silicon TO peak height, decrease rapidly from ~5.0 for uniform or large island samples to less than 0.02 for 5 µm islands. The ratio of SiGe TO peak height to silicon TO peak height is plotted as a function of island edge length in figure 3(b). The rapid decline in SiGe/Si PL intensity ratio with island size indicates that for small islands sizes, most carriers diffuse laterally in the SiGe after collection to recombine non-radiatively at surface defects on the exposed SiGe edges, and thus are not available for band-edge PL.

Model of edge recombination

The experimental results show that SiGe PL is being quenched by mid-gap states at island edges, as shown schematically in figure 4(a). To model the decrease in PL from carriers' diffusion to island edges, assume that PL from silicon occurs mostly in the substrate (i.e., not in the cap) and therefore that the silicon TO intensity is independent of island size. This assumption is justified because the absorption length of the PL laser (λ=514 nm) is approximately 340 nm, much greater than the thickness of the SiGe and silicon cap layers.

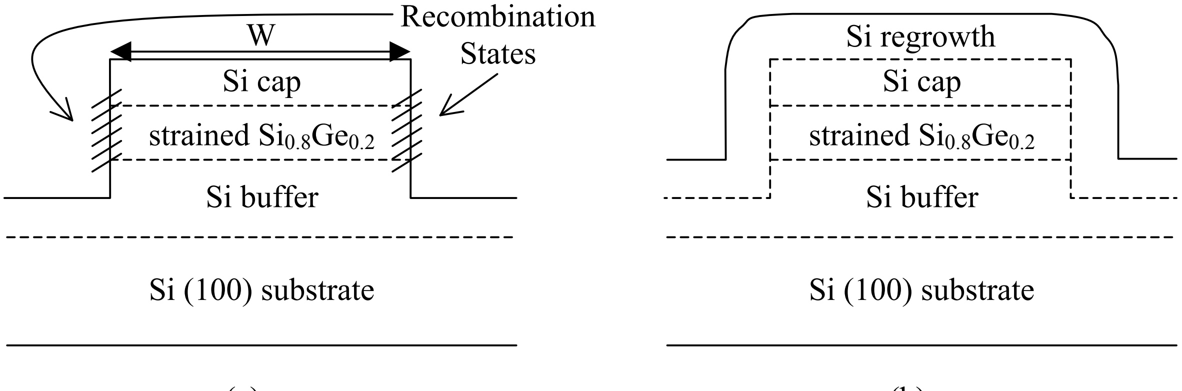
The SiGe photoluminescence strength, PL(W), as a function of the width of the island, W, is thus directly proportional to the excess number of minority carriers per unit length:

$$PL(W) = \frac{1}{W}\int_0^W n'(x)dx \,. \tag{1}$$



(a) (b)

Figure 3. (a) Photoluminescence of unpatterned and patterned 13 nm Si / 10 nm Si$_{0.8}$Ge$_{0.2}$ / Si for various island sizes. The PL intensity has been normalized to the silicon TO peak height. and (b) SiGe/Si PL intensity ratio vs. island edge length for unpatterned (solid line) and patterned (closed circles) samples. The vertical error bars are standard deviations of multiple measured values and the dashed line indicates the edge recombination model (see below.)



(a) (b)

Figure 4. Schematic cross-section of islands (a) with edge defects in SiGe and (b) with edges passivated by silicon regrowth.

The excess carrier concentration, n' = n - n_o, can be found from the solution of the one-dimensional steady-state carrier continuity equation under the condition of zero electric field

$$\frac{\partial n'}{\partial t} = 0 = G_{eff} - \frac{n'}{\tau} + D\frac{\partial^2 n'}{\partial x^2}, \tag{2}$$

which has the general solution

$$n'(x) = Ae^{x/L} + Be^{-x/L} + G_{eff}\tau, \tag{3}$$

where $L = \sqrt{D\tau}$. Here, G_{eff} is the effective generation rate, τ is the minority carrier lifetime, D is the minority carrier diffusion coefficient, and L is the minority carrier diffusion length in the SiGe. The “generation” is due to the capture of generated carriers in the SiGe from the underlying silicon, and is assumed independent of x. The coefficients A and B can be solved according to the appropriate boundary conditions, and the resulting equation for n'(x) used with Eqn. 1 to obtain PL(W).

For the case of infinite surface recombination, there are no excess carriers at the boundaries, n’(0)=n’(W)=0, and therefore

$$n'(x) = G_{eff}\tau\left\{1 + \left[\sinh\left(\frac{x-W}{L}\right) - \sinh\left(\frac{x}{L}\right)\right]\Big/\sinh\left(\frac{W}{L}\right)\right\} \tag{4}$$

and

$$PL(W) = G_{eff}\tau\left[1 - \frac{2L}{W}\tanh\left(\frac{W}{2L}\right)\right] \tag{5}$$

For the case of finite surface recombination velocity, S_n, the boundary conditions are

$$D\frac{\partial n'}{\partial x}\bigg|_{x=0,W} = S_n \cdot n'(x)\,. \tag{6}$$

In this case,

$$PL(W) = G_{eff}\,\tau\left\{1+\frac{L}{W}\left[A\left(e^{W/L}-1\right)+B\left(1-e^{-W/L}\right)\right]\right\} \tag{7}$$

where $A=\dfrac{S_n\tau+B\left(L+S_n\tau\right)}{L-S_n\tau}$ and $B=-\dfrac{S_n\tau\left[\left(L-S_n\tau\right)+\left(L+S_n\tau\right)e^{W/L}\right]}{2\left(L^2+S_n^2\tau^2\right)\sinh\left(W/L\right)+4S_n\tau L\cosh\left(W/L\right)}$. (8a, 8b)

The data in figure 3(b) was fit to the infinite surface recombination model (Eqn. 5) as shown by the dashed line. The SiGe/Si PL ratio of unpatterned samples gives $G_{eff}\tau$, so the only fitting parameter is L, the minority carrier diffusion length, which is found to be ~17 μm. This implies (assuming D=10cm^2/s) a lifetime in the SiGe of order of 0.3 μs.

Passivation of island edges by epitaxial silicon regrowth

In order to passivate the recombination states on the island edges, epitaxial silicon was regrown on top of patterned islands as drawn schematically in figure 4(b). A second set of samples is prepared as described above, but with a ~22 nm $Si_{0.8}Ge_{0.2}$ layer, and ~40 nm silicon cap. Arrays of islands are patterned on three pieces, with island edge lengths of 10, 30 and 100 μm, respectively. PL is measured for each island array and for an identical piece with no pattern. The samples are wet-cleaned with an HF-last process, and cleaned *in situ* with an 800°C, 10 Torr bake in hydrogen. Then, ~40 nm silicon is regrown at 700°C on the Si-SiGe-Si islands and on top of the piece with no pattern. After regrowth, PL is re-measured.

The PL intensity ratios as a function of island size are shown in figure 5, and the model parameters used to fit the measured data are listed in table I. The data taken before regrowth strongly resemble the results shown previously in figure 3(b) for similar samples. The data can be fit with the infinite surface recombination model, with a minority carrier diffusion length, L, of 26 μm, yielding a lifetime of 0.68 μs.

After silicon regrowth, the SiGe/Si PL ratio still decreases with island size, but it decreases less quickly than before. The slower drop of SiGe PL intensity as island size is reduced after silicon regrowth confirms that less recombination is occurring at the edge of the islands. The regrown silicon passivates some of the edge defects and thus increases the SiGe PL, but does not completely eliminate edge recombination, especially for the sample with 10 μm islands. The data is best fit using the finite surface recombination model derived above. G_{eff} and D are fixed at their values before regrowth. The unpatterned regrown sample can be fit with τ=0.50 μs and L=22 μm. (The reduction in diffusion length may be due to contamination introduced during the *in situ* clean and/or regrowth or gettered to the SiGe layer by the 800°C cleaning cycle.) The surface recombination velocity, S_n, is adjusted to fit the patterned sample data and found to be 4500 cm-s^{-1}.

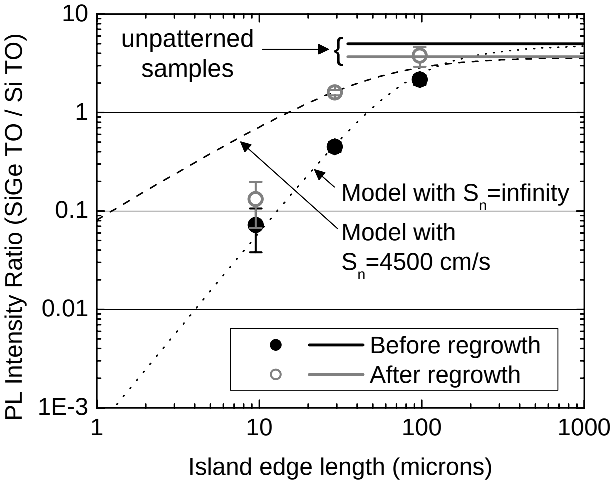


Figure 5. SiGe/Si PL intensity ratio vs. island edge length for samples before (closed circles) and after (open circles) silicon regrowth. The dashed lines indicate edge recombination model fits (see Table I).

	Before regrowth	After regrowth
D	$10\ cm^2s^{-1}$	
L	26 μm	22 μm
τ	0.68 μs	0.50 μs
S_n	∞	$4500\ cm\text{-}s^{-1}$

Table I. Parameters used to match infinite and finite surface recombination models to the silicon regrowth data shown in figure 5. L and S_n are the only fitting parameters.

CONCLUSIONS

Photoluminescence is a useful material characterization technique that can be readily applied to strained Si/SiGe layers used in advanced silicon technologies. If islands are used, the island edges may act as recombination sites, and thereby degrade the PL spectrum when the island size is comparable to or less than the minority carrier diffusion length. For our samples, this length is 15-30 μm, and SiGe PL peak heights from islands smaller than that are a factor of 100 times smaller than peaks obtained on unpatterned samples. For such small islands, the edge surface states can be partially passivated by epitaxial regrowth to increase the SiGe PL intensity. Minority carrier diffusion models have successfully been applied to fit the experimental data.

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