Temperature dependence of the indirect bandgap in ultrathin strained silicon on insulator layer

J. Munguía,[1,a)] J.-M. Bluet,[1] O. Marty,[1] G. Bremond,[1] M. Mermoux,[2] and D. Rouchon[3]
[1]*Institut des Nanotechnologies de Lyon (INL), CNRS UMR-5270, INSA-LYON, 7 Avenue Jean Capelle, Bat. Blaise Pascal, 69621 Villeurbanne, France*
[2]*Laboratoire d'Electrochimie et de Physico-chimie des Matériaux et des Interfaces, UMR 5631, (INPG–CNRS), BP75, 38042 Saint Martin d'Hères Cedex, France*
[3]*CEA, LETI, MINATEC Campus, 17 rue des Martyrs, 38054 Grenoble Cedex 9, France*

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Photoluminescence spectroscopy is applied on tensely strained silicon on insulator layer in order to evaluate the temperature dependence of the indirect energy bandgap. The strained silicon indirect bandgap follows a similar behaviour to bulk silicon at high temperature (from 80 K up to 300 K) which was described from the Varshni [Physica **34**, 149 (1967)] and Bose-Einstein equations. Nevertheless, at low temperature (from 9 K to 80 K), an unusual blueshift of the bandgap is evidenced. The latter can be modelled considering band-tail states of density of states which are related to the strain fluctuation. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.3691955]

Strained silicon (sSi) is one of the semiconductors which has been widely used as a channel in complementary metal oxide semiconductor (CMOS) technology because of strain induced electrons and holes mobility enhancement with respect to bulk Si.[1–3] The tensile strain induced in the sSi layers splits the sixfold degeneracy of the Δ_6 in Δ-direction in the conduction band into Δ_4 and Δ_2 valleys. The energy level of the two valleys (Δ_2) is lower than energy level of the four valleys Δ_4. Similarly at the Γ-point, the strain splits the valence band into light hole (LH) and heavy hole (HH) bands. The energy level of the LH band is higher than energy level of the HH. Thus, the electrons band (Δ_2) and the LH band settle the energy indirect bandgap of sSi. As a consequence, silicon (Si) indirect bandgap shrinkage is caused by the strain induced in the silicon layer; this effect predicted by theoretical calculation[4–6] has been confirmed in the previous works by low temperature photoluminescence.[7–9]

In this work, we report a photoluminescence study in order to evaluate the temperature dependence of the sSi indirect bandgap between 9 and 300 K with particular attention on the low temperature range (below 100 K). Even if these measurements may seem unnecessary for room temperature in CMOS technological application, they are fundamental for the understanding and the modelling of strained silicon on insulator (sSOI) electrical properties such as free carrier densities and mobilities extraction from temperature Hall measurements, for instance.

A silicon-germanium (SiGe) virtual substrate with grading Ge content up to 20% is used in order to induce strain in the overgrown silicon layer.[10] The 9 nm thick sSi layer as well as a few hundred nanometres of SiGe layer are transferred on a Si handle substrate using the Smart Cut™ process in order to obtain a SiGe/sSi/SiO_2/silicon substrate structure. Finally, a selective etching of the SiGe layer leads to a SiGe free sSOI wafer. A surface oxide layer has been realized in order to protect the sSi layer. This top oxide layer reduces the nonradiative surface recombination and then allows photoluminescence observation of the sSi layer. The photoluminescence measurements were carried out using the 363 nm UV line of an Ar+ laser and a Jobin-Yvon type HRS-2 monochromator in conjunction with a liquid nitrogen cooled Ge photodiode associated with a standard lock-in amplifier technique. The samples were placed in a cold stage which consists of a closed cycle He cryostat which enables measurements from 9 K up to room temperature. Micro-Raman spectroscopy in mapping mode has been performed using the 363 UV line of an Ar laser as excitation (resonant excitation with Si direct bandgap) and a Jobin-Yvon T64000 monochromator in a triple additive configuration. Low excitation power was used in order to prevent sample heating from the laser beam. Transmission electron microscopy (TEM) was performed on a Topcon EM002B electron microscope, working at 200 kV. Cross-section samples were thinned by mechanical thinning followed by ion milling.

In a previous work, we identified at low temperature a luminescence band at 0.983 eV as a transverse optical (TO) phonon assisted transition for a thin sSi layer which is 115 meV shifted towards low energy with respect to bulk Si transition.[7] The luminescence peaks as a function of temperature of the sSi sample and a bulk Si reference (Czochralski (CZ) n-type Si with 1 Ω cm resistivity) are shown in Figures 1(a) and 1(b), respectively. As the temperature increases from 9 K to 80 K, an unusual blueshift for the sSi peak is observed and at higher temperatures (80 K to 300 K), the emission shows a classical redshift. By contrast, the bulk Si spectra exhibit the well-known features of the near bandgap PL in Si.[11–13] In order to clarify the blueshift for the sSi sample at low temperature, we have reported in Figure 2 the evolution of temperature dependence of the sSi indirect bandgap energy which is compared to that of bulk Si. As an approach, we carried out the fit to our experimental data by using the Varshni empirical equation (dashed lines)[14]

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{(T+\beta)}. \quad (1)$$

a)Author to whom correspondence should be addressed. Electronic mail: jmunguia@ipn.mx.

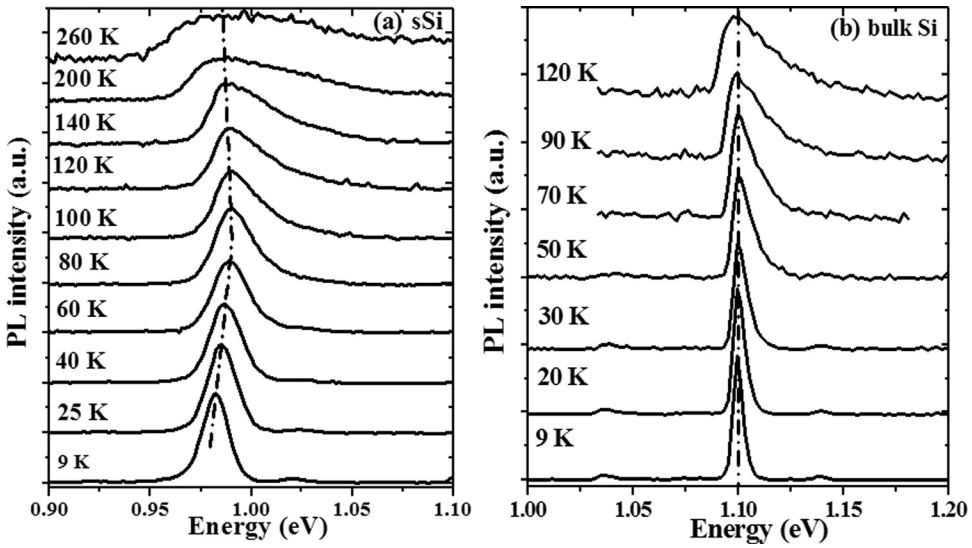

FIG. 1. Temperature evolution of the near band edge PL peak for (a) sSi sample and (b) bulk Si sample.

This equation is widely used to fit data by adjusting the parameters α and β. $E_g(0)$ is the energy bandgap at the temperature $T = 0$ K. In order to give better fits to the experimental data particularly for strained Si sample at low temperature, we have also fitted data by an alternative approach (solid lines) which had first been suggested by Viña *et al.*,[15]

$$E_g(T) = E_B - a_B\left[1 + \frac{2}{exp^{\left(\frac{\Theta}{T}\right)} - 1}\right]. \qquad (2)$$

This relation represents the modification of bandgap of a semiconductor due to the electron-phonon interaction at thermal equilibrium and may be derived from to Bose–Einstein approximation for the lattice vibration energy. Herein, the energy bandgap at $T = 0$ K is given in terms of the energy parameters E_B and a_B by the difference $E_g(0) = E_B - a_B$ and Θ represents an effective phonon temperature. A good fit to our experimental data is obtained for the bulk Si sample which exhibits a normal behaviour described by both models presented in Eqs. (1) and (2) as can be seen in Figure 2. However, for strained Si, even if a slight amelioration is seen with Viña *et al.* model, the blueshift of 8 meV observed between 9 K and 80 K cannot be described by both models.

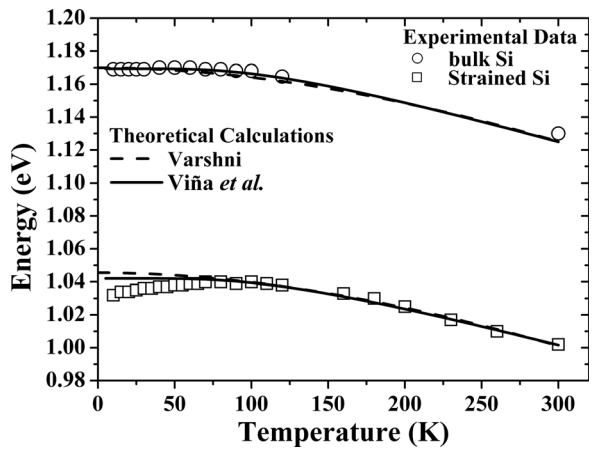

FIG. 2. Indirect bandgap variation (E_g) as function of temperature for bulk Si (circles) and strained Si (squares). The dashed and solid lines represent the fits using the Varshni and Viña *et al.* models, respectively.

Above 80 K, the strained Si bandgap dependence follows the same behaviour as the bulk Si one. The fit resulted in the parameter values reported in the Table I. The parameter values related to the strained Si sample agree with the ones obtained previously for bulk Si via the same models.[14,15]

The change of the energy bandgap with temperature is a result from the change in bond lengths with temperature and can be related to the pressure coefficient of the energy bandgap through the compressibility and the thermal expansion coefficient. In order to improve the fit in the sSi sample experimental data specially at low temperature, we realized an additional correction taking into account the bulk Si negative thermal expansion coefficient at low temperature.[16–18] However, this parameter has a very slight effect on the bandgap energy but this is insufficient to improve significantly the experiment-theory correlation in our case.

As can be observed in the Figure 2 and discussed above, the temperature dependence of the strained Si indirect bandgap does not follow the monotonic variation of the Eqs. (1) and (2) at low temperature. Similar behaviour has previously been observed in quantum well structures for III-V materials[19–21] as well as in superlattices of II-V1 materials.[22] It was proposed that the luminescence in these materials originates from the recombination of excitons localized at potential fluctuations. The anomalous temperature-induced emission shift is attributed to the band-tail states in density of states (DOS) which is due to a certain degree of disorder occurring mainly at interfaces, which may be of compositional and/or structural origin. In the frame of this model at

TABLE I. Values of the parameters E_g, α, and β obtained by fitting the temperature dependence of indirect bandgap in strained Si from the Varshni equation and E_B, a_B, and Θ parameters from the Viña *et al.* equation.

	Varshni model			Viña *et al.* model			
Sample	$E_g(0)$ (eV)	$\alpha \times 10^{-4}$ (eV/K)	β (K)	$E_g(0)$ (eV)	E_B (eV)	a_B (eV)	Θ (K)
Bulk Si	1.169[a]	7.021[a]	1108[a]	1.169[b]	1.218[b]	0.049[b]	349.7[b]
Strained Si	1.066	7.0	1120	1.063	1.111	0.048	365

[a]Values from Ref. 14.
[b]Values from Ref. 15.

lower temperature (9 K), the sSi excitons do not have sufficient thermal energy to overcome potential barriers and become trapped in adjacent lower energy levels of the DOS where the recombination takes place. The blueshift of 8 meV is then a result of the thermal population of higher energy states of the DOS. Here, a transition from the localized states in the strained Si takes place. Above 80 K, the strained Si energy bandgap indicates that the carriers are fully delocalized. Then the bandgap follows a classical redshift.

A model which has been proposed by Bergman *et al.*[23] is used in order to explain the blue temperature-induced shift in strained Si luminescence. The model is based on band-tail filling of a Gaussian DOS with a standard deviation parameter σ which describes the dispersion of density of states (i.e., its width) and $E_D(T)$ is attributed to the energy range between the center of the Gaussian DOS of the electrons and that of the holes. This leads to the following simple expression of the bandgap variation with temperature:

$$E(T) = E_D(T) - \frac{\sigma^2}{k_B T}. \tag{3}$$

In addition, the model assumes that $E_D(T)$ depends on temperature in the same manner as the gap energy (without DOS) and thus $E_D(T)$ can be described via Varshni model (Eq. (1)) and Viña *et al.* model (Eq. (2)). We use the model proposed by Bergman *et al.* in order to explain the variation of the strained Si energy bandgap as well as to estimate the extent of the DOS. The fitting result is presented in Figure 3, using both Eqs. (1) and (2) for $E_D(T)$ variation. A good fit is evidenced for the strained Si experimental data at low temperature. The deduced density of state dispersion (σ) is around 5.7 meV when using Eq. (1) and 4.8 meV when using Eq. (2).

In order to gain further insight into the mechanisms determining the recombination of the strained Si layer, the temperature dependence of the integrated luminescence intensity was investigated. The inset of Fig. 3 presents the temperature dependence of the PL amplitude $I(T)$ which was fitted (solid line) according to the relation,[24,25]

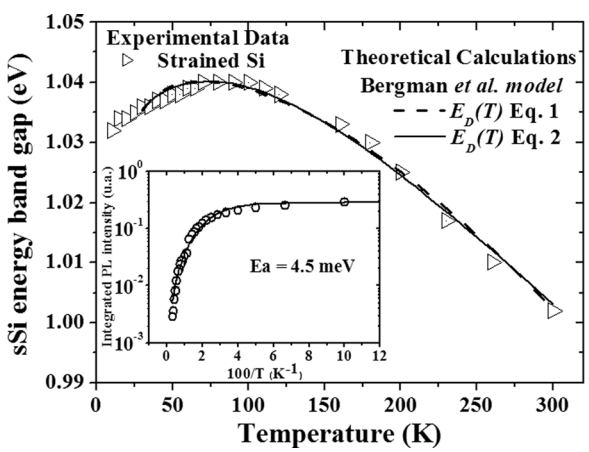

FIG. 3. Temperature dependence of strained Si indirect bandgap. The lines represent the fit by Bergman *et al.* model described from Eq. (3), considering for $E_D(T)$, Varshni equation (dashed line), and Viña *et al.* equation (solid line). The inset depicts the integrated PL intensity evolution as a function of temperature.

$$I(T) = \frac{I_0}{1 + gT^{\frac{3}{2}} exp\left(\frac{-E_a}{k_B T}\right)}, \tag{4}$$

In this relation, I_0 is the PL intensity at $T = 0$ K, E_a is an activation energy, k_B is the Boltzmann constant, T is the temperature, and g is a fitting parameter.[24] An activation energy $E_a = 4.5$ meV was ascertained from the fit. This E_a value agrees quite well with the one obtained for the energy width of the DOS (σ). Thus, this activation energy (4.5 meV) can be interpreted as the energy that carriers need in order to overcome potential barriers (4.8 meV–5.7 meV). The states in the band tails are formed in local potential minima, resembling quantum dots. Their origin could be assigned to various causes, such as composition fluctuations (for compound semiconductor), high density of impurity states, inhomogeneous lattice deformations, and surface roughness. We show in Figure 4(a) a cross-section transmission electron micrograph of the sSOI structure. It reveals no evidence of interface disorder which could be responsible for potential fluctuation and the carried localization. Nevertheless, some contrast modulation within the strained Si layer which could be related to strain modulation is observed. This strain modulation is clearly evidenced from Raman spectroscopy mapping. Indeed, in Figure 4(b) which shows a $50 \times 50\ \mu m^2$ mapping image of Si-Si mode Raman shift in strained Si, bright and dark bands are seen to run along ⟨110⟩ direction, which reflects the strain fluctuation. Using deformation potential from literature,[26,27] the average strain deduced from the global shift in comparison to the bulk Si-Si mode position (521 cm^{-1}) correspond to the expected 0.8% for a Si layer grown on a 20% Ge content SiGe layer. The maximal fluctuation of Raman shift in Figure 4(b) is 0.5 cm^{-1} corresponding to a maximal (peak to peak) strain fluctuation of 8%. This value is a quite good agreement with the 4.5% strain fluctuation which can be deduced from low temperature PL considering the 5 meV standard deviation deduced from Bergman *et al.* model versus the global strain induced shift of the bandgap of 115 meV.

In summary, photoluminescence was used to analyze the temperature dependence of strained Si indirect bandgap in sSOI structure. A blueshift was observed in strained Si bandgap at low temperature (from 9 K to 80 K). A band-tail-filling model with a Gaussian DOS distribution was proposed to explain the blue temperature shift of sSi energy bandgap and verifying the existence of a defect density of states in the recombination of excitons at low temperatures. This carrier

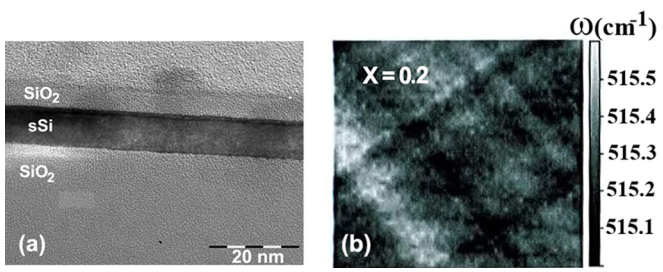

FIG. 4. (Color online) (a) Cross section TEM image taken under high resolution conditions from sSi sample and (b) Raman mapping image of the Si-Si mode in the strained Si layer.

localized at low temperature has been correlated to strain fluctuation in the sSi layer which can be determined by this way in good agreement with micro-Raman mapping results.

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