Characterization of High Quality RTCVD Relaxed Si_{1-x}Ge_{x} Grown on Ge Graded Buffer Layers on Si by Photoluminescence Spectroscopy

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Relaxed Si_{1-x}Ge_{x} layers grown by rapid thermal chemical vapor deposition (RTCVD) have been characterized by photoluminescence (PL) spectroscopy. The structures consist of a Si_{1-x}Ge_{x} capping layer with a 0.32 and 0.52 Ge concentration, grown on a compositionally graded Si_{1-x}Ge_{x} buffer layer. The effect of the composition grading rate on the layer quality has been intensively studied. Well-resolved near band edge luminescence (excitonic lines with no-phonon and phonon replica similar as in bulk SiGe alloys) coming from the relaxed alloy capping layer and dislocation-related bands (D1, D2, D3, D4 lines) in the graded buffer layer have been measured. The electronic quality of this relaxed capping layer, controlled by the design of the compositionally graded buffer layer, has been determined by the excitonic photoluminescence. A detailed analysis of the energy of the D4 dislocation band demonstrates that the main misfit dislocations remain confined in the first steps of the graded buffer layer. Si_{1-x}Ge_{x} layers grown on these pseudo-substrates either under compressive or tensile strain and the well-defined PL results obtained are discussed on the bases of strain symmetrization and of high quality of the layers. This points out the possibility of using such high quality relaxed Si_{1-x}Ge_{x} layers as substrates for the integration of new devices associated with Si technology.

**Key words:** Photoluminescence, RTCVD, SiGe

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**INTRODUCTION**

The emergence of lattice-matched pseudo-substrate corresponding to the fabrication of high quality relaxed Si_{1-x}Ge_{x} layers should allow to develop novel electronic and optical device applications needing of strain engineering. This should give the opportunity to monolithical integration of different semiconductor materials. A defect-free substrate with an adjustable lattice parameter between the Si and Ge ones would enable the development of many new electronic and optical devices within the Si technology framework. Fully relaxed thick SiGe buffer layers grown with a uniform Ge content allow a too high density of dislocations (typically $10^8$–$10^{10}$ cm$^{-2}$) to propagate which is not compatible with the good operation of devices. The original concept of the virtual substrate introduced by Kasper et al.$^{1}$ consisting of a partly relaxed thin SiGe buffer layer and improved by Presting et al.$^{2}$ for the fabrication of ultrathin Si$_m$Ge$_n$ superlattices, has to be used very carefully and needs the knowledge of growth and thermal stability conditions. The major purpose of these substrates is to allow the growth of Si or SiGe films under tensile strain. Such a strain gives rise in pseudomorphically grown Si or SiGe layers to the type II band alignment required for the confinement of electrons in a two-dimensional gas at the Si/SiGe heterostructure used in n-modulation-doped field-effect transistor (MODFET) channel transistors. Another important possibility is to use the strain symmetrization concept to grow very thick active Si$_m$Ge$_n$...
short period superlattices. These superlattices are in full development for optoelectronic device applications. The buffer layer plays a key role since it controls the strain and growth quality of the lattice mismatched epitaxial film and thus its electronic properties.

Improvements in obtaining low densities of threading dislocations by growing a compositionally graded SiGe buffer using molecular beam epitaxy or chemical vapor deposition have recently been reported. This graded buffer has been proved to result in a threading dislocation density three to four orders lower than the uniform buffer layer ones. In this context, a very recent study has shown lower threading dislocation densities (in the 10⁴–10⁵ cm⁻² range) by using rapid thermal chemical vapor deposition to grow totally relaxed compositionally graded SiGe buffer layers at high temperature with low grading rate. Due to the slow Ge increase, the strain in the buffer never reaches a value where a high density of threading dislocations can nucleate to the detriment of the increase in length of misfit dislocation segments.

As a characterization technique, photoluminescence (PL) spectroscopy is very well adapted to measure the radiative recombination of defects such as dislocations and to control the electronic quality of such pseudo-substrates. PL studies have recently been reported on molecular beam epitaxially (MBE) grown compositionally graded SiGe buffer layers, testing the viability of PL spectroscopy for nondestructive characterization. Using the same experimental techniques, aimed at investigating the electronic quality of the material, this paper reports a systematic PL characterization on the low dislocation densities rapid thermal chemical vapor deposition (RTCVD) pseudo-substrate already described in Ref. 5.

**EXPERIMENTAL PROCEDURES**

The samples are grown by RTCVD in a four inch single wafer reactor (Jipelec FUV4) formerly described. Each sample, a four inch Czochralski <100> silicon wafer, is chemically cleaned before loading and subsequently hydrogen baked in situ at 1020°C for 30 s. A 160 nm silicon buffer layer is first grown at temperature from 900 to 950°C and then cooled down to 820°C for the SiGe alloy growth. Typical silicon epitaxial growth conditions are: total pressure of 200 Pa with a 2 slm hydrogen carrier flow and 40 sccm of silane (slm and sccm denote liters per minute and cubic centimeters per minute, respectively, at standard temperature and pressure); a mixture of 10% germane is added into hydrogen for SiGe alloy growth. The buffers studied in this work consist of a compositionally graded layer (the composition increasing from 12 to x at% Ge) capped with a uniform Si₁₋ₓGeₓ layer. Buffers without any uniform capping layer were also grown and investigated. The grading rates used are in the 3–48% Ge per µm range, the cap layer is 1.1 µm thick and the final composition x is typically 32% but demonstrations up to 52% were also carried out. A single-step 32% SiGe layer has been grown for comparison with graded buffer layers.

The PL measurements are carried out using the 514.5 nm line of a cw argon-ion laser with power densities ranging from 1 to 50 W/cm². The samples are strain-free mounted on a copper block and placed in a variable temperature, He gas, steady-flow cryostat allowing PL measurements from 4.2K to room temperature. The PL signal goes through a high-resolution grating monochromator (Jobin Yvon-type HRS2) and into a liquid-nitrogen-cooled high-sensitivity Ge p-i-n detector (Applied Detector Corporation). The emission signal is processed by a conventional lock-in technique.

**RESULTS AND DISCUSSIONS**

**Comparison of Uniform and Graded Buffer Layers**

Figure 1 shows the comparison of the PL spectra measured at 4.2K for the uniform steep buffer layer (with x₀ = 0.32) with a compositionally graded "pseudo-substrate" (12% Ge/µm). The uniform buffer layer exhibits the well-known D (D₁, D₂, D₃, D₄) PL lines attributed to the recombination process related to the dislocations in the SiGe layers. Their energy at the maximum intensity shifts vs the Ge content as reported by Weber and Alonso. Luminescence from the Si substrate can also be observed. No luminescence