Spectroscopic ellipsometry of Si_xGe_{1-x} / Si : a tool for composition and profile analysis in strained heterostructure used in the microelectronics industry.

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Si_xGe_{1-x}/ Si strained -layer hetero structures play a primary role in the Si-based fast electronics developments of today. Real time epitaxial growth control of this alloy as well as *ex situ* on line characterization of the processed wafers is required. Indeed, among other techniques, spectroscopic ellipsometry (SE) corresponds to a fast and non-destructive one as compared to SIMS and/or XRD analysis. Ellipsometric studies of heterostructure-base-transistor (HBT) , with either graded or abrupt profiles are reported. The analysis is based on optical databases of indices currently provided in the literature for relaxed material. Within the case of strained pseudomorphic structures, using a calibration procedure to access the real x alloy composition, the in-depth variation x can be determined even with the presence of a silicon capping layer. Good results are obtained for dummy load test wafers as well as for patterned processed wafers where to analyze areas such small as 30x30 microns is needed. This work has been carried out within the *GRESSI* consortium between *CEA-LETI* and *France TELECOM-CNET.*

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1. Introduction

The *Si_xGe_{1-x} / Si* strained-layer heterostructure plays an important role in band-gap engineering and Si-based fast electronics device applications such as HBT transistors and optoelectronic devices [1,2]. The classical tools employed for composition determination, excepting x-ray diffraction (XRD) and optical interference Nomarski observations, are all destructive, (i.e., Rutherford backScattering spectroscopy (RBS), cross-section transmission electronic microscopy (XTEM) and Secondary Ions Mass Spectroscopy (SIMS) [3-5]. Furthermore, in the microelectronics industry, the control of the growth parameters, needs perfect adjustment to insure the right x composition and a perfect crystalline structure, (dislocations free), while keeping a complete good spatial uniformity, even in the case of the new generation of 12 inches (300 mm) diameter silicon wafers. An optical non-destructive system in line can achieve this goal as a real time supervising tool. For instance, an optimized linear graded layer is to be monitored by ellipsometry while, e.g., the germane GeH_4 flow rate inside the growth reactor [6] is smoothly varying. The Ge composition and graded linear profile are usually being only inspected *post deposition* only by SIMS [7] simply because the other methods fail because the lack of abrupt composition interfaces due to the graded layer. As a *non-destructive* method, *in situ* real time spectroscopic ellipsometry (SE), i.e., within the cluster tools reactor chamber, has been already used to control epitaxial growth process [8]. Now, SEs are among the list of available clean room environment characterization tools in ULSI factories and are in the roadmap of the next 300 mm Si wafers tools generation[9]. Under this pressure, an intensive instrumental development began from SE suppliers to provide a fast acquisition time (few milliseconds per Ψ and Δ ellipsometry angles spectra), while keeping accuracy, repeatability, and a small spot size probe (~30x30microns). Software also is evolving increasing its capability [10]. SE with a variable incidence angle is complementary, enabling eliminate ambiguities between correlated parameters, also assessing physical models. In a previous paper [11], it is described how the epitaxial growth of Si_xGe_{1-x} can be studied considering the physical phenomena present in these structures. It is shown hereafter how the models can be implemented as usable recipes in an industrial SE software. In this case, the output from the instrument imperatively needs being fast, together with an easy and direct determination of stack characteristics, (thickness, slope of the linear profile together with the epitaxial alloy composition.

2. SE Measurements.

Several SE $Si_{1-x}Ge_x$ studies, without graded layer, have already been reported in the literature [10-18]. A didactical example is given in Fig. 1. There, SE measurements are reported for the case of graded-composition layer with a very thin silicon cap. SE has been carried out for several incidence angles Φ using a home-built Fourier analysis, photon-counting rotating-polarizer SE. In Fig. 1, SE measurements correspond to symbols (Φ=74 to 78 degrees) and the best-fit model results are represented by continuous lines for tanΨ and cosΔ, the classical ellipsometric parameters, versus photon energies in electron volt, eV. Increasing incidence angles Φ shifts the onset of the Brewster transition toward higher photon energies, the upper thin silicon cap and the Si_xGe_{1-x}/Si interfaces generates slight optical interference modulation, although damped by the x graded layer and only seen in the cosΔ variation. These details can be magnified and revealed only with the variable angle technique. It is relevant in the near infrared range although being more or less damped, depending on the abruptness of the graded layer. This behavior is typical of heterostructures, as the one schematically depicted in the inset fig.1-a. Thickness and composition parameters can then be extracted from the fitting model with SE data.

At the Helium Neon laser wavelength, n and k have an approximately linear behavior versus the x composition in this composition range[18,19]. The optical indices n, k profiles are similar to the in-depth composition profile, (see refs.12 and 18). The corresponding depth profiles of the optical constants n and k at 1.96ev, deduced from data processing are also shown in 1-b. In the blue part of the visible spectral range, where the critical points (CP) singularities are located, occurs a red shift following the x alloy composition. The E_1, $E_1+\Delta_1$ optical transitions from the conduction band to the valence bands, fall within the 3.4 eV (Si, i.e., 0%Ge) and 1.8eV (100% Ge, x=0) range [20].

The database or look-up table model.

From previous measurements, optical indices for several alloy x composition have been reported in the literature for bulk material [19], or for thick (several microns thick) unstrained films [21] or even strained layers [12]. With these results a database table, for any x composition, can be built using the alloy mixing algorithm [22] to model the optical indices n, k at any wavelengths. The absolute x values, deduced from other methods (SIMS or XRD), have been compared with those obtained from SE for both relaxed and strained SiGe. Reductions in x of the order of 0.03 have been observed, e.g., in Refs. 12 and 17. when strained films are compared with relaxed ones, ellipsometry measurements revealed the effect of strains induced by the lattice mismatch between the silicon substrate and the layer. A smaller alloy composition value is the consequence of the strain present in the Si_xGe_{1-x} layer [12-18]. In many previous works the discrepancies between absolute x composition (as obtained from SIMS analysis) and the SE alloy x composition, interpreted as coming from the effect of strains, were seen to be the reason of failure of this method. Indeed, the refraction index is determined by intrinsic parameters, density and atomic polarisability and macroscopic phenomena such as strains. The refraction index (n), at 1.96 eV, of strained epitaxial Si_xGe_{1-x} films on silicon has a smaller value than for relaxed or unstrained film. The difficulty to incorporate stresses has been underlined by many authors. No refined model including both strain and alloy composition has been proposed yet although it is definitely highly needed.

Then the only approach is to correlate the results between SE with SIMS or XRD [11]. The absolute x values can be estimated directly from SE, and used in the case of the industrial SE characterization. A first step when studying strained alloy graded epi-layer samples is to build a "matched" database with samples reference and then use SE analysis.

Linear graded HBT

In the HBT, the addition of Si_xGe_{1-x} into the base region of a Si bipolar transistor (with x graded concentration) speeds electron conduction across the base region by reducing the

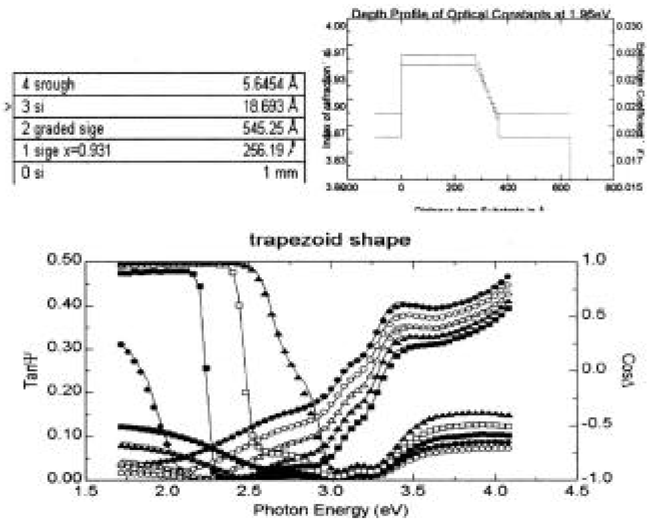

Fig. 1 Didactical graded sample (trapezoid profile) and SE measurements. Symbols and best fit model (lines) for Ψ and Δ versus wavelength and several incidence angles (Φ=74 to 78 degrees) in the case of the 12%Ge, HBT strained Si_xGe_{1-x} /graded Si_xGe_{1-x}/ Si structure. In the inset , are schematically depicted the corresponding model and the plot of the respective n and k corresponding depth profiles extracted from SE.

band gap and creating a ramped potential surface (drift field). In fact strain is used to engineer the band gap. An optical index profile has to be accounted for when a linear graded concentration is employed in a device. The general multi layer optic model is obtained by slicing into n_l sub layers the Si_xGe_{1-x} graded layer in such manner that the composition of each sub layer follows a linear law. For the Si_xGe_{1-x} graded layer one have

$$x(d)=d*(1-c)+c \quad \textit{or} \quad x(d)=(c-1)*d+1 \qquad (1)$$

for a downhill linear slope or an up-hill slope respectively. Here, d is a parameter varying between 0 and 1 across the layer thickness. A number of 3 to 5 sub layers are sufficient when describing this linear profile. It makes the regression analysis fast enough without involving additional parameters. The c parameter of equation (1) is constrained to be equal to the concentration x of the preceding (or following), alloy layer in the stack. During that work, test were accomplished for the case of triangular and trapezoidal graded profile shapes (as shown in figure 1). A perfect correlation has been found with the SIMS profiles.

A look-up table can be build with very narrow composition steps to insure accuracy in the range of interest and in order to reduce the computing time, using the alloy mixing algorithm [22], and starting with one of the known published database, i.e., composition x versus $Si_{1-x}Ge_x$ optical data,. This table can be then incorporated in the analysis software of the, for instance, industrial KLA TENCOR 1280SE [23].

3.Microelectronics Applications: Uniformity deposition control in a process environment

Index and x composition profile determination

In figure 2 the case of a patterned wafer where the structure is a composition step graded $Si_{1-x}Ge_x$ 20nm-thick sample is shown. The targeted compositions were respectively 10,20,30,20,10 %Ge steps Si_xGe_{1-x} layer 20nm thick and an additional Si capping layer 20nm-thick. The structure is shown in figure 2-a together with the decomposition process used in the composition-graded model. The figure 2-b and c represent respectively the curve fitting result between experiment and the computation, and the optical profiles for n, k at 632.8 nm versus thickness. These measurements were made with a 30 x 30 µm light beam spot size at 71.5 degrees incidence angle.

Spatial homogeneity and Mapping

In Fig 3 we shown two three-dimensional (3D) graphs of SE 49 pints mapping measurements of Si_xGe_{1-x} /Si-capped thickness, x=0.9, using the KLA-TENCOR 1250SE. The upper 3D profile , corresponds to the Si cap whereas the bottom one, corresponds to the Si_xGe_{1-x} layer. Even with the two thickness layers obtained from the same Ψ, Δ measurements, no correlation between them is noticeable. The global shape is due to a lack of uniformity over the susceptor temperature. The different deep amplitudes seen in the middle of the two layers thickness plots are due to a the specific growth rate of Si and $Si_xGe_{1-x,}$ the respective Si and Si_xGe_{1-x} deposition rate activation energies are different, higher in Si than in the alloy, a weak temperature related non-uniformity is more important in the Si capping

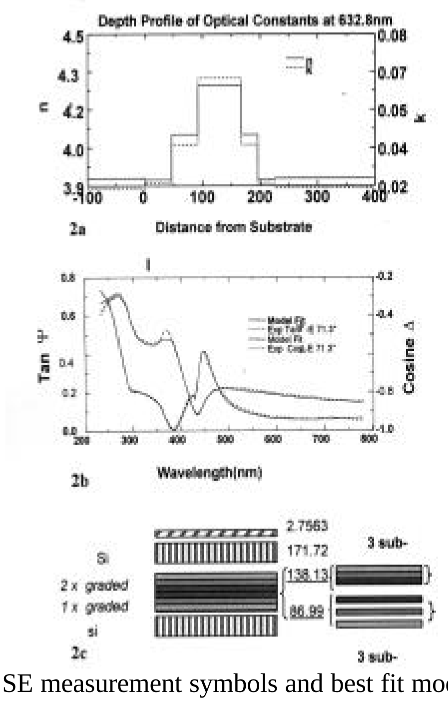

Fig 2 a. SE measurement symbols and best fit model (lines) for Ψ and Δ versus wavelength and in the case of a respectively targeted 10,20,30,20,10 %Ge steps structure 20nm-thick of strained Si_xGe_{1-x} capped with a 20nm thick Si layer. Experimental data and simulated curves are reported in 2b.The mulitlayer model is depicted. In 2

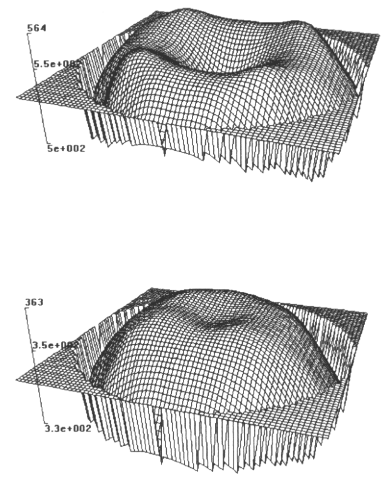

Fig.3 3-Dimensional mapping of the Si_xGe_{1-x}/ Si structure measured, in an industrial SE tool through 49 points polar map: upper, Si capping 3D map; bottom, SiGe.

layer than in the Si_xGe_{1-x} layer. In fact, the same ΔT enhances more the Si than the SiGe growth process.

4.Conclusions.

In the case of Si_xGe_{1-x} / Si heterostructures, SE analysis for different incidence angles can solve both composition and profile in the HBT graded layers specifically when the incidence angle Φ is around or higher than the Brewster angle for Si. In this case, a linear alloy composition slope can be detected otherwise the problem remains for low incidence angle with somewhat correlated parameters.

A method of how to use the unstrained optical index literature databases in order to estimate right compositions, have been described. Due to strain, a calibration correlated with the absolute parameters of growth has to be accomplished. From these results, it is shown that using a look-up table algorithm, even in a linear graded layer model, an industrial SE instrument, with a very small spot size probe, can be of the great interest. Beside profile determination, the growth conditions in the reactor can be adjusted, e.g., the susceptor geometry in the epitaxy reactor allowing to enhance the spatial uniformity.

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