

Strain measurements of a Si cap layer deposited on a SiGe substrate determination of Ge content

Raman spectroscopy is one of the most popular tools for investigating the basic properties of semiconductors. It is particularly efficient in establishing the characteristics of microelectronic devices because the performance of SiGe based devices highly depend on the knowledge of the composition, Ge content and the strain of the layers.

Indeed, the ability to measure alloy composition and strain in semiconductor structures is essential for the calibration of growth processes and control of the electrical and optical behaviour of these materials.

The first requirement for the study of mechanical stress with Raman spectroscopy is that the investigated material exhibits Raman active modes, ie that there is a well defined Raman band in the spectrum. These include materials such as diamond, silicon, SiGe, InGaAs, GaAs, GaN, to name a few.

Mechanical strain directly affects the frequency positions of the Raman modes and can lift their degeneracy. Typically, it is possible to observe and detect strain by analysing the shift in the band position, but it can also affect the band shape and induce broadening and deformation of peaks. These effects depend upon the material characteristics and on the stress and strain geometry.

The typical structure of the sample (named sample 1) studied here is shown in figure 1.

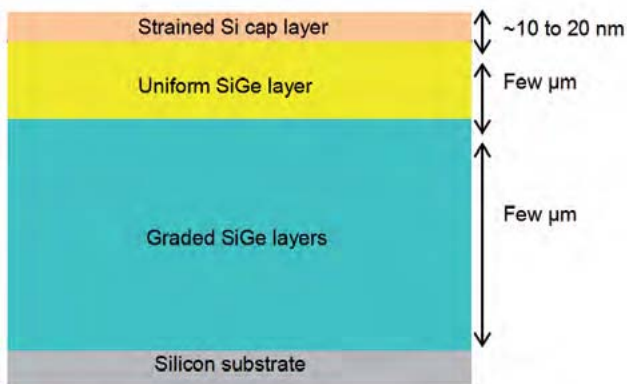


Figure 1 : Typical structure of Si/SiGe/Si sample

In this study, we will focus on the choice of the laser excitation and measurement conditions. Results obtained in the visible and in the UV range will be presented.

Influence of the laser

The choice of the laser excitation will influence different parameters :

- The signal collection, because the Raman intensity is directly proportional to $(1/\lambda)^4$.
- The probing volume that depends on the laser spot size and the beam penetration.
- The level of fluorescence that may overwhelm Raman signal.
- The resonance effect where there is strong wavelength dependence of some Raman bands.
- The coverage and resolution since the grating dispersion varies along the spectral range.

For strongly absorbing materials such as many semiconductors, the Raman signal originates from a volume defined by the penetration depth and the diameter of the laser beam. A shorter laser wavelength gives rise to lower penetration and therefore provides information on the strain closer to the surface.

Different penetration depths in silicon and germanium are given for different wavelengths in the table below.

Laser wavelength (nm)	Penetration depth in Si (nm)	Penetration depth in Ge (nm)
633	3000	32
514	762	19.2
488	569	19
457	313	18.7
325	~10	~9
244	~6	~7

Figure 2 : Table of penetration depths in Si and Ge influence of the excitation wavelength

The commonly used visible excitations limit the spatial discrimination in both lateral and axial dimensions. UV micro Raman can greatly enhance the spatial resolution by taking advantage of the shorter wavelength and much smaller optical penetration depth. For example, one can reduce the focused laser spot size from 0.7 μm to 0.45 μm by changing the laser line from 514 nm to 325 nm using an X100 objective with a NA of 0.9.

Moreover, the much shorter optical penetration depth in the UV (~ 10 nm at 325 nm in Si) allows probing shallow active layers.

The effect of the laser selection is illustrated in figure 3 that shows the spectra recorded at different wavelengths on the sample described in figure 1.

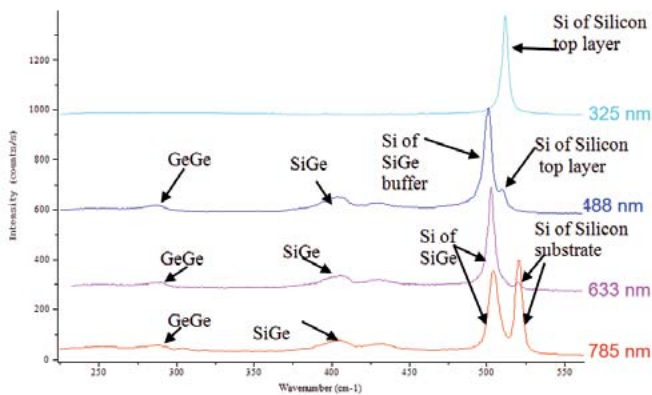


Figure 3 : Spectra recorded at 325, 488, 633 and 785 nm on sample 1

Interest of combining visible and UV investigations

Because of their different penetration depths, combining visible and UV measurements can be of great interest for samples with a structure such as described in figure 1. At the end of this note, the technique used to separate the effects of composition and strain will be discussed.

Measurement conditions

In terms of experimental definition and instrumental set up, several parameters have to be considered in order to optimise the accuracy and reliability of the information. To start with, the determination of the peak position can be improved by using a reference band. Indeed, this will allow one to remove the influence of external parameters such as environmental temperature that can also affect the frequency of the monitored Raman peak. Ideally this reference should be acquired simultaneously with the Raman band. This is why the plasma lines from the laser source itself are usually very well suited as they provide sharp emission of well known frequency that are collinear with the Raman spectra. Spectra will then be corrected with respect to the plasma position.

The use of an autofocus device is also of great importance. Optimising the focus manually can induce an artificial variation of the position of the plasma lines, due to differences in illumination of the entrance slit of the spectrograph. Therefore on the one hand the autofocus function allows one to maintain proper illumination and guarantee the plasma position and on the other hand, it enables one to correct for any sample tilt or surface roughness.

Finally, one physical factor that can affect the measurement of stress is the localized heating of the sample. If the laser power density at the sample is too high, it is possible to heat the sample at the point of focus. This results in a temperature induced down-shift of the Raman peak.

For this reason, it is generally recommended to run with low laser powers, typically at a sub mW level.

Results

Visible Raman spectrum.

The samples were characterized by using the 488 nm line of an Argon laser.

At 488 nm, due to the penetration effect mentioned before, the spectrum is dominated by the signal coming from the SiGe layer.

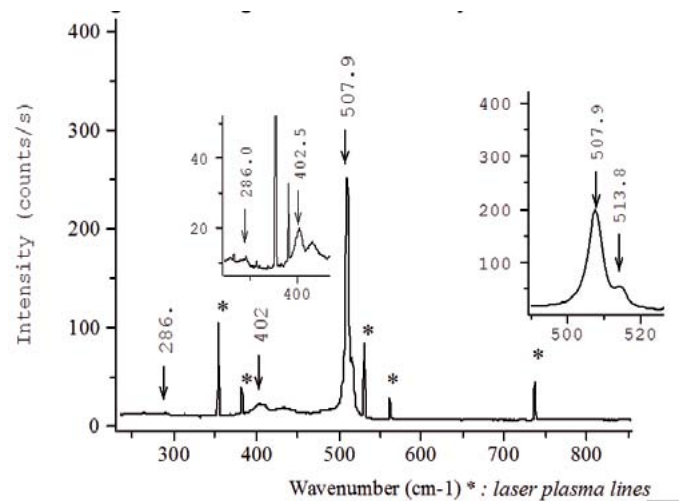


Figure 4 : Raman spectrum acquired at 488nm

Inspection of the spectra indicates that it is difficult to obtain precisely the positions of the SiGe and GeGe modes due to the larger width, asymmetric shape and the weaker intensity of these lines. But the higher the signal to noise ratio, the better the precision will be on the position of the SiGe and GeGe bands.

UV Raman spectrum

The figure below shows the spectrum of sample 1 recorded at 325 nm.

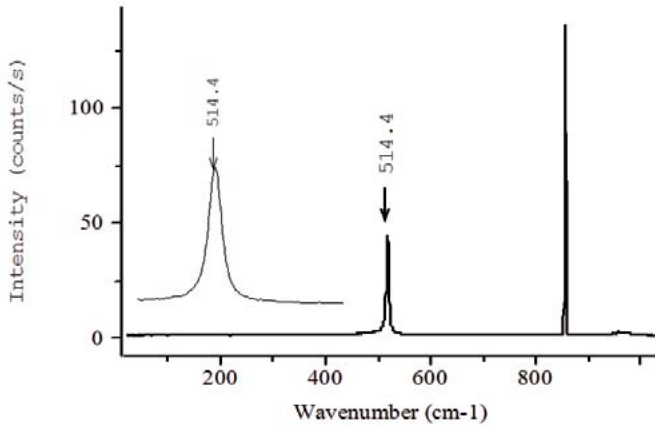


Figure 5 : Raman spectrum acquired at 325 nm

In the visible spectrum (fig.4) the bands of the SiGe layer are dominant. The peak of the Silicon cap layer is visible although it appears as a shoulder. Hence it is difficult to determine precisely its position.

If we refer to the different penetration depths of various laser lines for the silicon material, we can see that the value in the UV range is a few nanometers. Therefore to study thin silicon layers, the use of UV excitation line is a solution. As a consequence the UV spectrum of sample 1 shown in fig. 5 only shows the silicon peak of the thin top layer and can be used to define the position of the Silicon line ω_{Si} from this cap layer.

Correlation of spectroscopic data with sample composition and strain

From the visible Raman spectrum we can get the position of the SiSi and SiGe modes of the SiGe layer.

In 1989, based on a linear interpolation of low and large Ge concentration, Alonso [1] estimated the correlation of Ge content (x) to the SiSi phonon peak position ω_{SiSi} for thick layers of relaxed SiGe alloy to be defined by the formula

$$\omega_{SiSi} = 520.0 - 68x$$

Tsang [2] reported that for thinner layers and values of x close to 0.3, the formulae become :

$$\omega_{Si} = 520.2 - 62x \quad \text{equation 1}$$

$$\omega_{SiGe} = 400.5 + 14.2x \quad \text{equation 2}$$

Formulae have also been developed taking into account the strain ϵ [4]:

$$\omega_{SiSi} = 520.2 - 62x - 815\epsilon \quad \text{equation 1b}$$

$$\omega_{SiGe} = 400.5 + 14.2x - 575\epsilon \quad \text{equation 2b}$$

$$\omega_{GeGe} = 282.5 + 16x - 385\epsilon \quad \text{equation 3b}$$

The result of calculations based on these formulae gives the Ge content and strain or degree of relaxation, based on the Raman spectrum of the film. These formulae can be applied for visible excitation Raman spectra.

In the case of UV spectrum recorded from the cap layer of sample 1, the peak shift is measured relative to the unstrained bulk silicon and this value is then used to evaluate the degree of strain as discussed above.

Conclusion

Raman spectroscopy is a very well suited technique to determine both Ge fraction and strain in SiGe layers and Si cap layers.

Moreover the possibility of using both UV and visible excitation lines on the same instrument is essential to study structures made up of a Silicon cap layer on top of a SiGe layer. The relative Ge content in the constant $Si_{1-x}Ge_x$ layer is calculated from the visible Raman spectrum and the strain of the cap Si layer is derived from the UV Raman spectrum.

References

- [1]M.L. Alonso, PhD, thesis, University of Stuttgart, Stuttgart (1989).
- [2]Tsang et al, Measurement of alloy composition and strain in thin $GexSi_{1-x}$ layers, J. Appl. Phys. 75 (12), 15 June 1994.
- [3]Leroy, et al, New Industrial solution for measuring Strain and Ge content on sSi and SiGe wafers using Raman spectroscopy, Semicon west 2004.
- [4]Chen et al, Physical review B, Volume 65, 233303