Non-destructive Characterization of Ge Content and Ge Depth Profile Variations in $Si_{1-x}Ge_x/Si$ by Multi-wavelength Raman Spectroscopy

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A multi-wavelength, micro Raman spectroscopy system was designed and used for non-contact and non-destructive thickness and Ge content characterization of $Si_{1-x}Ge_x/Si$. The thickness and Ge content estimated by Raman measurements were compared to those values obtained from X-ray diffraction (XRD) and X-ray reflectance (XRR) measurements for cross-reference and showed very good agreement. The multi-wavelength excitation capability of the Raman system allows non-contact and non-destructive probing of Ge concentration as well as Si stress in $Si_{1-x}Ge_x/Si$ along the depth direction. The Ge concentration gradient of small size test pads (as small as 10μm x 10μm) in depth direction were successfully measured using the multi-wavelength Raman system. The multi-wavelength Raman system with high spectral and spatial resolution is found to be very attractive and powerful for characterizing advanced semiconductor materials, such as $Si_{1-x}Ge_x/Si$ and strained Si. It is also very useful for monitoring and controlling process equipment and process conditions.

Introduction

Strained Si and strained $Si_{1-x}Ge_x/Si$ with enhanced electron and hole mobility are widely used in high speed complementary metal-oxide-semiconductor (CMOS) and heterojunction bipolar transistor (HBT) devices [1-6]. The Ge content and thickness of a $Si_{1-x}Ge_x$ layer of the $Si_{1-x}Ge_x/Si$ determines the amount of strain and the degree of electron and hole mobility enhancement. Carrier mobility enhancement in strained Si, as well as in strained $Si_{1-x}Ge_x$, is strongly dependant on the magnitude of strain in the channel region and can be modulated by controlling the Ge content. Accurate measurements of strain and Ge content are extremely important for process optimization and precise manufacturing process control. However, the electrical property enhancement of device performance in strained Si and strained $Si_{1-x}Ge_x/Si$ can be measured only after the completion of the metallization process. For effective process optimization and quality control, it is important to establish non-destructive and in-line $Si_{1-x}Ge_x/Si$ characterization and monitoring techniques.

Microscopic Raman scattering is a powerful, non-destructive technique for characterizing crystallinity, the degree of stress or strain of the crystal and Ge content in $Si_{1-x}Ge_x$ [3-7]. For this purpose, intensity, Raman shift, and full width at half maximum (FWHM) of Raman signals corresponding to Si and $Si_{1-x}Ge_x$ are measured. By selecting an appropriate excitation wavelength, probing depth of Raman measurement can be selected [8-14].

Conventional Raman spectroscopy systems are limited in their effectiveness by repeatability and stability issues, as well as distortion, resolution and an inability to make measurements at exactly the same spot with depth profiling. To overcome these common issues with conventional Raman systems with a single excitation wavelength, we have designed a multi-wavelength Raman spectroscopy (MRS-300) system as an in-line stress/strain and Ge content monitoring system which can obtain information at different depths. Additionally, to improve the accuracy, consistency and usefulness of the MRS-300, it was designed with no moving parts and a minimum of optical components for improved stability and repeatability, and a longer focal length for enhanced spectral resolution [8-10]. Preliminary results on the performance of the newly designed Raman system (MRS-300) and Raman characterization of mechanically stressed Si and $Si_{1-x}Ge_x$/Si were reported previously [9].

In this paper, we have demonstrated non-contact and non-destructive characterization of the thickness and Ge content in $Si_{1-x}Ge_x$/Si using the MRS-300 system in a highly accurate and repeatable manner. An example of an in-line Ge content monitoring application of the MRS-300 system is provided.

Experiment

Element and alloy semiconductor materials, including Si, $Si_{1-x}Ge_x$/Si and Ge have their own spectral responses depend on lattice parameters, energy band structure, impurity, defects and surface conditions, among other things. Light with photon energy greater than the bandgap of a semiconductor is partially absorbed and partially reflected when directed at the semiconductor surface. The rate of intensity attenuation in the depth direction is higher for the shorter wavelength (higher photon energy). The absorption coefficient is higher for light with shorter wavelength (higher photon energy) and the penetration depth is shallower. The light penetration depth (or probing depth) of Raman characterization can be adjusted by selecting appropriate excitation wavelengths and this characteristic can be utilized for depth profiling.

We have designed the MRS-300 system as an in-line stress/strain monitoring system. The system has three thermoelectrically cooled, charge coupled device (CCD) cameras that can measure Raman signals from three different excitation wavelengths without any disruption (i.e., without scanning the monochromator or switching the excitation laser). The schematic illustration and measurement capability of the system are summarized in Fig. 1. Three major spectral lines (457.9, 488.0 and 514.5nm) from a multi-wavelength Ar^+ laser are used as the excitation source. By selecting the wavelength of the excitation laser, the crystal quality, stress and strain in the depth direction can be characterized [8-14].

A stress-free blanket Si (100) wafer was prepared as a measurement reference. A large number of epitaxially grown $Si_{1-x}Ge_x$/Si (100) wafers with different Ge content and different $Si_{1-x}Ge_x$ layer thickness were prepared and Raman signals from them were measured under three different excitation wavelengths. The Ge content of $Si_{1-x}Ge_x$ layer was varied from 15 to 35 atomic percent. The thickness of the $Si_{1-x}Ge_x$ layer was varied in the range of 30 nm ~ 120 nm.

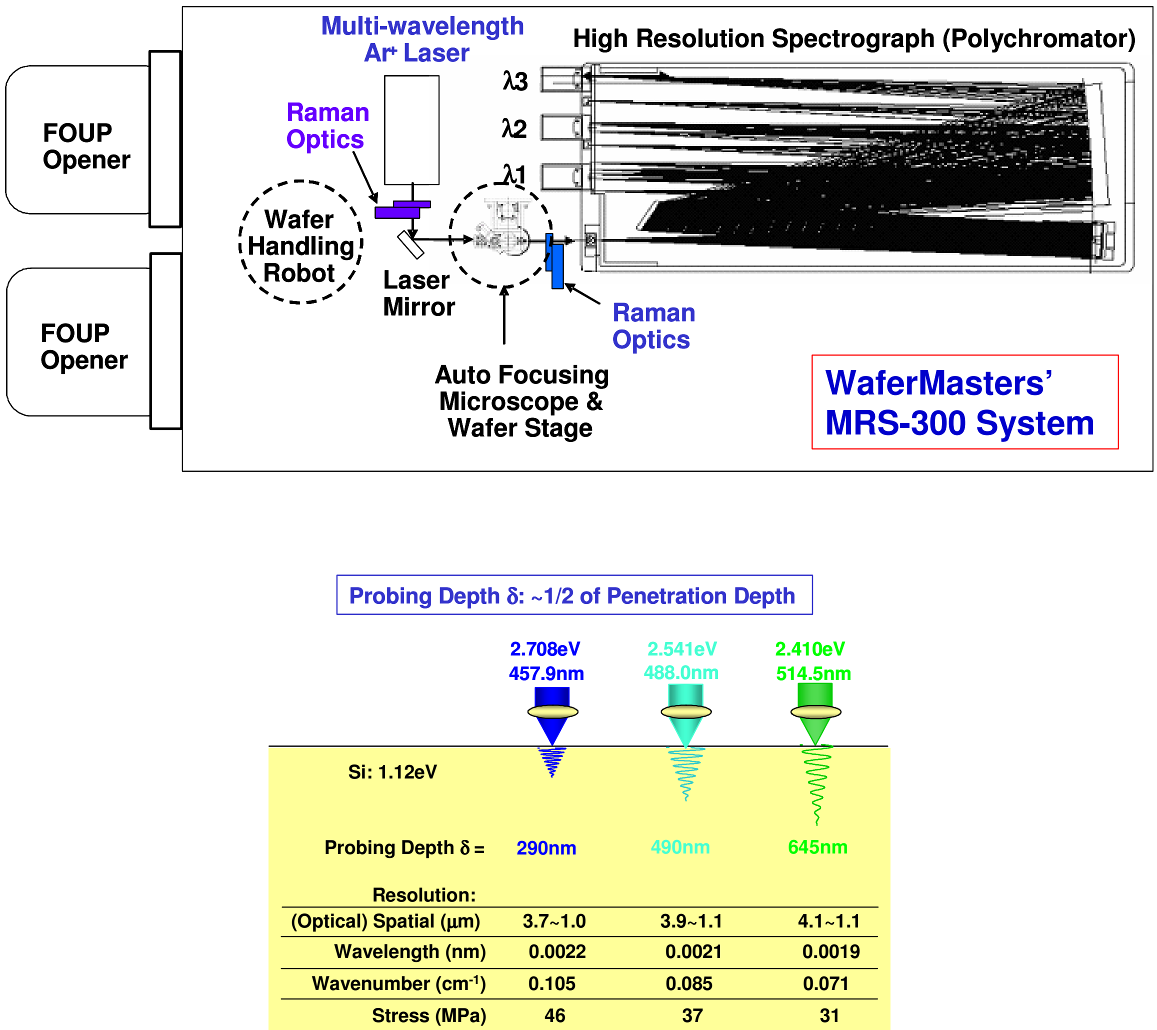


Figure 1. Schematic illustration of multi-wavelength Raman spectroscopy (MRS-300) system and summary of measurement capability.

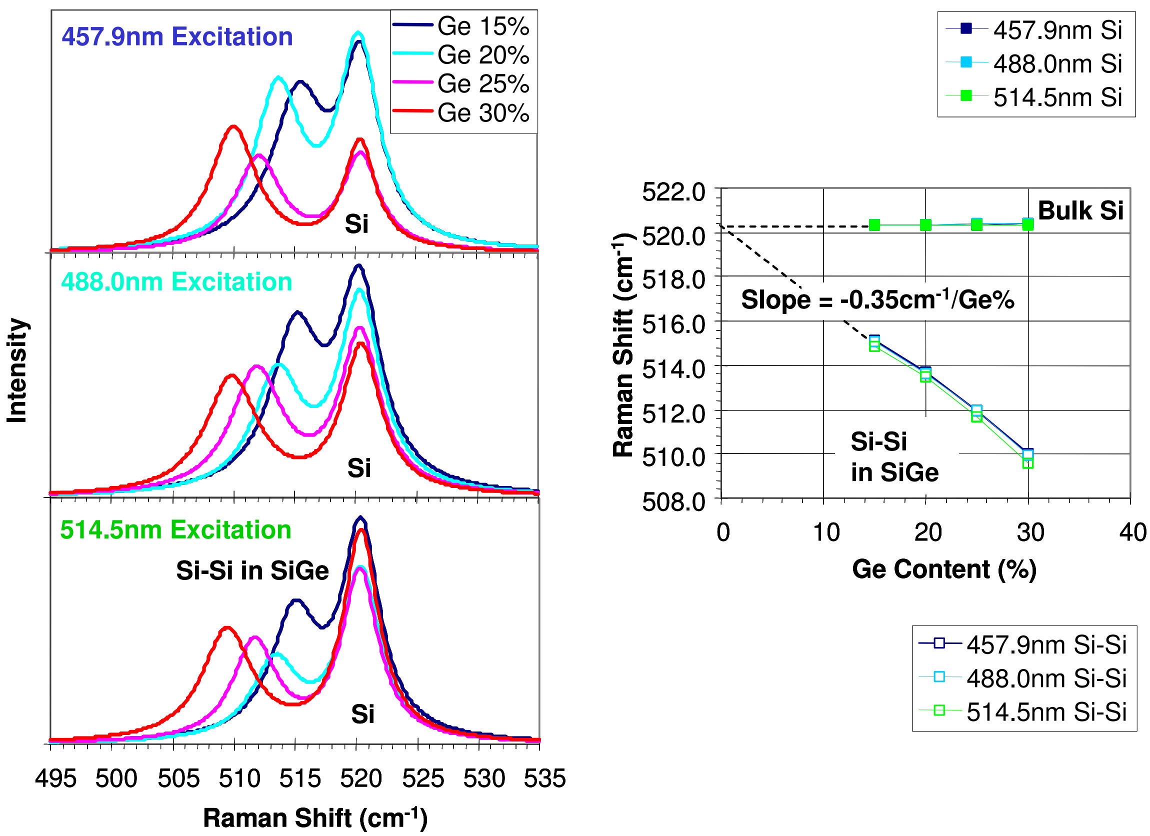
RESULTS AND DISCUSSIONS

In conventional monochromator-based Raman systems, frequent system calibration (a few times a day) is required under normal operating conditions. When the excitation wavelength is switched, additional calibration and system stabilization time (of up to several hours) is needed before meaningful data acquisition. However, the unique, no-moving part design of the MRS-300 system was able to minimize the uncertainties in the absolute wavenumber of Raman signals due to calibration errors and optical misalignment due to vibration and backlash of moving parts (mainly diffraction grating(s)), common mechanical problems in conventional Raman systems. The MRS-300 system design made multi-wavelength Raman measurements from the same measurement site possible without refocusing or calibrating between switching of excitation wavelengths for different probing (penetration) depths. This innovative design feature of the MRS-300 has significantly improved the reliability of Raman measurement and made the in-line monitoring of properties of Si (stress, strain, Ge content, $Si_{1-x}Ge_x$ layer thickness etc.) possible for process development, optimization and quality control.

Measurement repeatability of the MRS-300 system was tested using a stress free blanket Si (100) wafer for a period of three months. Variations in Raman shift and FWHM at all three excitation wavelengths during the three month testing period was less than $0.05cm^{-1}$. Reliable high resolution Raman studies and in-line monitoring of stress, strain and the effect of Ge in $Si_{1-x}Ge_x$ became possible.

Raman signals from a large number of $Si_{1-x}Ge_x$/Si (100) wafers with different Ge content, ranging from 15 to 35 atomic percent and different $Si_{1-x}Ge_x$ layer thicknesses ranging from 30nm to 120nm were measured using the MRS-300 system under 457.9nm, 488.0nm and 514.5nm excitation. As seen in Fig. 2 (a), all four $Si_{1-x}Ge_x$/Si (100) wafers with different Ge content, showed a second peak, on the left (the lower wavenumber side) of the (reference) Raman peak from bulk Si at $520.3cm^{-1}$, regardless of excitation wavelength. The second peak is identified as a Raman signal from Si-Si bonds in $Si_{1-x}Ge_x$. As the Ge content increases, the second peak, from the Si-Si bonds in $Si_{1-x}Ge_x$, shifts towards the lower wavenumber side. This phenomenon is well known and the separation of the second peak of $Si_{1-x}Ge_x$ from the bulk Si peak is often used to determine the amount of strain and/or Ge content in $Si_{1-x}Ge_x$ [3-6, 18]. As the $Si_{1-x}Ge_x$ layer thickness increases, the intensity of the second peak from Si-Si bonds becomes stronger and intensity of the bulk Si signal becomes weaker. From the intensity ratio (I_{Si-Si}/I_{Si}) of the Si-Si signal to the bulk Si signal, at a given excitation wavelength, the thickness of the top $Si_{1-x}Ge_x$ layer can be estimated. For thin $Si_{1-x}Ge_x$ films on Si, Raman signals from the shorter excitation wavelength, with its shallow probing (penetration) depth should be used for accurate $Si_{1-x}Ge_x$ film thickness estimation. Only one peak from the Si-Si bond in the $Si_{1-x}Ge_x$ layer is observed with Raman measurement of thick $Si_{1-x}Ge_x$ layers on a Si wafer under the shorter excitation wavelength. This is because the shorter excitation wavelength cannot reach the Si wafer through thick $Si_{1-x}Ge_x$ top layer. For film thickness estimation on a thick $Si_{1-x}Ge_x$ film on Si, Raman signals from the longer excitation wavelength, with a deep probing (penetration) depth, should be used.

The positions of Raman peaks for bulk Si and Si-Si bonds in $Si_{1-x}Ge_x$ layers of various Ge content are plotted in Fig. 2 (b) as a function of Ge content in atomic percent. As seen in Fig. 2 (b), a monotonic increase of the separation of the second peak of $Si_{1-x}Ge_x$ from the bulk Si peak occurs at a rate of $-0.35cm^{-1}$/Ge atm% at all three excitation wavelengths [9, 14]. Ge content measurement values were in good agreement with the Ge content measured by high resolution x-ray diffraction (HRXRD), within measurement error (<0.1 atm%). By measuring the separation between the bulk Si peak and Si-Si peak from $Si_{1-x}Ge_x$ layer, non-contact and non-destructive characterization of stress and/or Ge content of $Si_{1-x}Ge_x$ can be accomplished in-line from either blanket or patterned wafers. By virtue of its repeatability, Raman measurements of wafers between process steps can be used as a process quality assurance method as well as for important inputs for process development, optimization and qualification. Variations in Raman peak positions (shifts), FWHMs and separation between the two peaks can provide immediate feedback of strain and/or Ge content variation within a wafer and wafer-to-wafer. Raman measurement results under different excitation wavelength also provide the same valuable information in the depth direction. In Fig. 3, the Raman peak intensity ratio of I_{Si-Si}/I_{Si} in $Si_{0.72}Ge_{0.28}$/Si (100) under various excitation wavelengths is plotted as a function of $Si_{0.72}Ge_{0.28}$ layer thickness. The thickness of $Si_{0.72}Ge_{0.28}$ layers was compared to x-ray reflectance (XRR) measurement data.



(a) (b)

Figure 2. Si and Si-Si Raman peaks from $Si_{1-x}Ge_x$/Si (x = 0, 0.15, 0.20, 0.25 and 0.30) wafers under 457.9nm, 488.0nm and 514.5nm excitations.

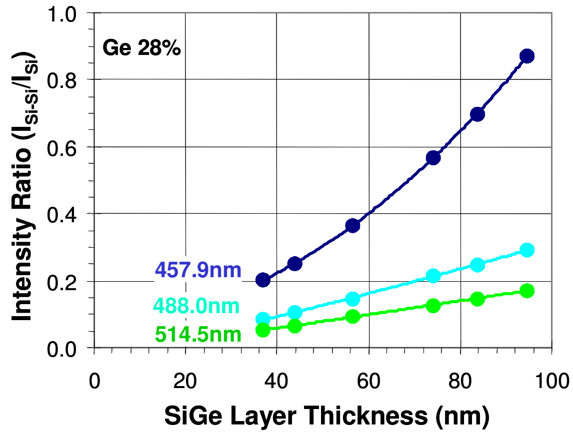


Figure 3. Raman signal intensity ratio of I_{Si-Si}/I_{Si} measured from $Si_{0.72}Ge_{0.28}/Si$ (100) samples with various $Si_{0.72}Ge_{0.28}/Si$ layer thicknesses under different excitation wavelengths.

Ge content measurement of $Si_{1-x}Ge_x/Si$ test pads with various dimensions (300µm x 300µm ~ 0.25µm x 0.25µm) was attempted using the MRS-300 system. Ge content measurement values were very consistent in test pads with sizes down to 10µm x 10µm. Figure 4 shows multi-wavelength Raman spectra measured from a small test pad (10µm x 10µm) on a device wafer. As seen in the figure, Raman spectra, from all three excitation wavelengths, have two peaks, one strong peak from the Si wafer and one weak peak from Si-Si bonds in $Si_{1-x}Ge_x$. The position of the weak peaks from the Si-Si bonds in $Si_{1-x}Ge_x$ shows a monotonic shift towards the lower wavenumber side as the excitation wavelength increases (greater penetration depth). Each Raman spectra was deconvoluted into two peaks (assumes symmetric Lorentz distribution). Deconvoluted peaks were plotted along with raw data. The estimated Ge content from the Si-Si peak position after deconvolution was in the range of 30.5 atm% ~ 33.0 atm%. Based on the multi-wavelength Raman spectra, the $Si_{1-x}Ge_x$ layer has a Ge gradient in depth direction. The top layer has smaller Ge content and Ge content increases towards the $Si_{1-x}Ge_x/Si$ interface region. The derived Ge content and gradient was in good agreement with $Si_{1-x}Ge_x/Si$ epitaxial condition and other characterization results using HRXRD and secondary ion mass spectroscopy (SIMS) data. Due to the non-contact and non-destructive nature of Raman measurements, the MRS-300 system can be used as an in-line process and material characterization tool for both blanket and patterned wafers.

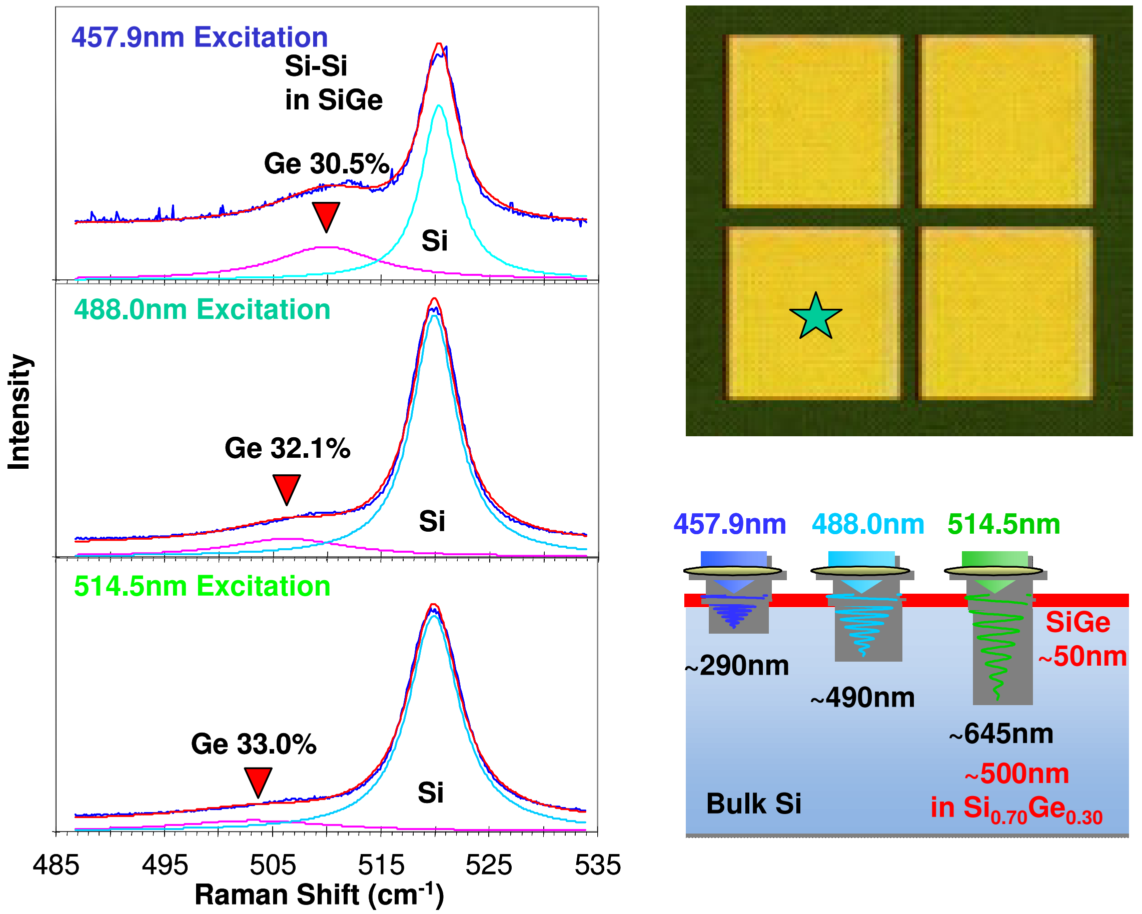


Figure 4. Raman spectra from a small test pad (10µm x 10µm) of $Si_{1-x}Ge_x/Si$ measured using MRS-300 system under various excitation wavelengths.

Conclusions

A polychromator-based multi-wavelength Raman spectroscopy system (MRS-300) is introduced for non-destructive, material and process characterization applications of semiconductor materials such as Si, $Si_{1-x}Ge_x$ and Ge. The unique design features of the MRS-300 system are reviewed and their effects are described in comparison with the common issues with conventional Raman measurement systems. The performance of the MRS-300 system and non-destructive nature of lattice stress/strain and Ge content characterization were introduced as application examples. The applications of the MRS-300 for in-line process monitoring of Ge content and $Si_{1-x}Ge_x$ film thickness were introduced and the measurement results were compared with ones from HRXRD and XRR measurements. Successful measurement of Ge a concentration gradient on small size test pads (as small as 10µm x 10µm) in the depth direction was introduced. The MRS-300 system with very a high wavenumber resolution, high measurement repeatability and depth profiling capability is proven to be very useful as an in-line process, material and equipment monitoring tool.

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