Depth Profiling of Si/Si_{1-x}Ge_{x} Structures by Micro-Raman Imaging

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1. Introduction
It is well known that tensile stress in Si films of Si/Si_{1-x}Ge_{x} structures raises carrier (hole/electron) mobility in the Si films [1]. Strained silicon (s-Si) technology for high speed devices has been investigated extensively because of its possibility to overcome deadlock coming from so-called scaling technique in miniaturizing individual devices. Quantitative characterization of physical properties of the Si/Si_{1-x}Ge_{x} is earnestly desired for architecting s-Si devices. Raman measurements have been widely used for evaluation of crystallinity and Ge composition for Si/Si_{1-x}Ge_{x} heterostructures [2-6]. Recently, we have reported Raman analyses of cross sections of Si/Si_{1-x}Ge_{x} heterostructures using a line illumination method [6]. The cross sectional Raman measurements, however, were not enough to obtain depth profiles of strain and Ge composition in thin Si_{1-x}Ge_{x} graded layers.

Raman imaging using angle lapping of Si/Si_{1-x}Ge_{x} structure is expected to improve the depth resolution. In this study, we report detailed depth profiles of Si/Si_{1-x}Ge_{x} structure inspected by means of Raman scattering using several excitation sources and beveled structure of Si/Si_{1-x}Ge_{x} composites.

2. Experiments
The sample used in this study was commercially available one grown by chemical vapor deposition. Schematic description of the Si/Si_{1-x}Ge_{x} structure is given in Fig. 1. A Si_{1-x}Ge_{x} buffer layer (3.0 µm, x=0.2) was deposited on a graded Si_{1-x}Ge_{x} layer (2.2 µm, 0≤x≤0.2) on a Si (001) surface. An active Si layer (17.5 nm) was deposited on the Si_{0.8}Ge_{0.2} buffer layer. The specimen was angle-lapped at an angle of 1° with respect to the surface. The beveled surface was mirror finished by chemomechanical polishing. When we use the beveled specimen, the depth resolution is expanded by 1/sin(1°) ≈ 57.3 times. Raman scattering measurements performed using the 364 and 488 nm lines of an argon ion laser as excitation sources. Difference in the penetration depths of the excitation light for Si and/or Si_{1-x}Ge_{x} alloy makes depth profiling of Si/Si_{1-x}Ge_{x} layers possible. One-dimensional micro-Raman imaging of the Si/Si_{1-x}Ge_{x} structure was made by line illuminations of the 488 nm laser beam which was expanded with a cylindrical lens mounted in front of a microscope and focused linearly (10×370 µm²) on the sample surface. Ordinary point illuminated macro-Raman measurements were also performed with the 364 nm line. Raman spectra were obtained at intervals of 3.5 µm by successively moving the sample in the direction perpendicular to the bevel edge with a stage. A diameter of the 364 nm laser spot on the sample surface was about 50 µm. Raman measurements were performed in near backscattering geometry. Scattered light was dispersed with a 1 m double monochromator and detected by a liquid nitrogen cooled charge coupled device (CCD) detector.

3. Results and Discussion
Depth profiles of the Si/Si_{1-x}Ge_{x} structure were obtained by Raman measurements. Figure 2 (a) shows Raman spectra obtained by the point illumination with the 364 nm line and Fig. 2 (b) shows a Raman image obtained by the line illumination with the 488 nm line. These Raman profiles correctly reflect the sample structure depicted in Fig. 1. The Raman signal of the s-Si layer could not be detected in Raman imaging excited by the 488 nm line because the penetration depth of the 488 nm excitation light is larger than thickness of the top s-Si layer. On the other hand, the Si band of the top s-Si layer is clearly detected by the 364 nm excitation as shown in Fig. 2 (a). The penetration depth of the 488 and 364 nm lines for Si is 300 and 5 nm, respectively [2]. Spatial resolution in depth of micro-Raman measurements with the 488 nm excitation is limited by the penetration depth of the laser light. For the macro-Raman measurement with the 364 nm excitation using the beveled specimen, the spatial resolution in depth was ~ 400 nm at present. However, micro-Raman technique with the 364 nm...
excitation will improve the spatial resolution in depth to better than 20 nm. Peak frequencies and FWHMs of the Si-Si bands of the s-Si on top and Si$_{0.8}$Ge$_{0.2}$ buffer layers, which were obtained by Lorentzian function fits to data, are plotted in Fig. 3. Uniformity of tensile stress of the s-Si layer and variation of x in the Si$_{1-x}$Ge$_x$ alloy can be analyzed from the peak frequencies shown in Fig. 3 (a) and (b).

Lateral positions in Fig. 2 were converted into depth parameters in Fig. 3. As clearly shown in Figs. 3 (a) and (b), the FWHM of the Si-Si band of the Si$_{1-x}$Ge$_x$ graded layer has two maxima. The broadening of the Si-Si band indicates presence of many defects. The slope of the frequency vs. depth curve shows that the grading of Ge concentration is not uniform in the Si$_{1-x}$Ge$_x$ graded layer. The grading is gentle in the middle of the graded layer where the FWHM has a minimum. High density of defects would be intentionally induced in the graded layer by the rapid grading. In addition, good crystallinity of the Si$_{0.8}$Ge$_{0.2}$ buffer layer can be inferred from the FWHMs which approach to FWHMs of the Si substrate. Introduction of the high density of defects in the graded layer would be beneficial to reduce the number of threading dislocations and bring the full strain relaxation in the Si$_{0.8}$Ge$_{0.2}$ buffer layer [7]. The frequency of the Si-Si band in the buffer layer is 506.5 cm$^{-1}$. This is very close to the frequency of the Si-Si band (506.3 cm$^{-1}$) of a Si$_{0.8}$Ge$_{0.2}$ alloy whose strain is assumed to be completely relaxed [6]. The in-plane strain of the s-Si layer was estimated to be 0.77% from the frequency of the Si band [5]. The details of the estimation have been presented in Ref. 6.

We have studied a Si/Si$_{0.8}$Ge$_{0.2}$ layer/Si$_{1-x}$Ge$_x$ graded layer/Si structure by Raman scattering measurements. The depth profile of the Si$_{1-x}$Ge$_x$ graded layer was obtained in high spatial resolution by Raman measurements with multiple excitation sources and angle-lapped structure. In-plane stress of the top s-Si layer was estimated by UV Raman measurements. The present results demonstrate that micro-Raman imaging with beveled structure and UV excitation sources is a powerful tool for analyzing Si/Si$_{1-x}$Ge$_x$ structure.

References