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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(1º) ≈ 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 μm^2) 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 35 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.

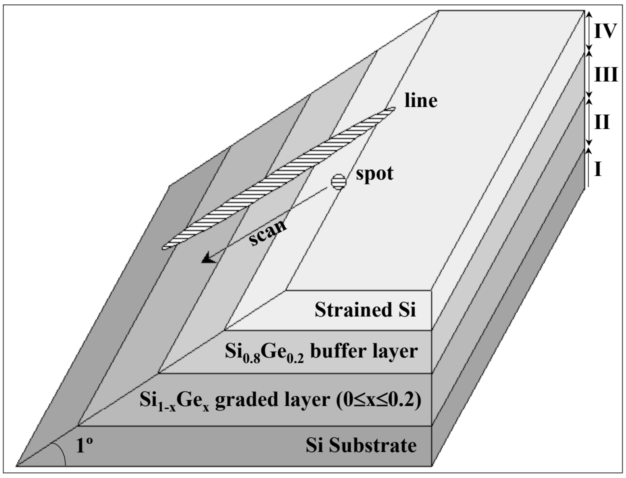

Fig. 1. Schematic description of a $Si/Si_{1-x}Ge_x/Si$ sample: (II)=2.2 μm, (III)=3.0 μm, (IV)=17.5 nm.

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).

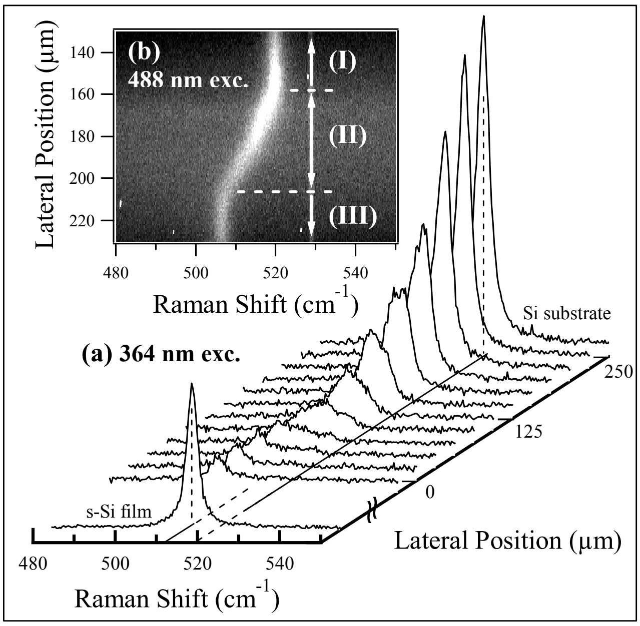

Fig. 2. (a) Raman spectra of a beveled $Si/Si_{1-x}Ge_x$ sample obtained by point illumination with the 364 nm line. (b) A Raman image of the same sample obtained by line illumination with the 488 nm line. (I): Si substrate, (II): graded $Si_{1-x}Ge_x$, (III): $Si_{0.8}Ge_{0.2}$ buffer layer. Note that the origin of the lateral positions in (a) does not correspond to that in (b).

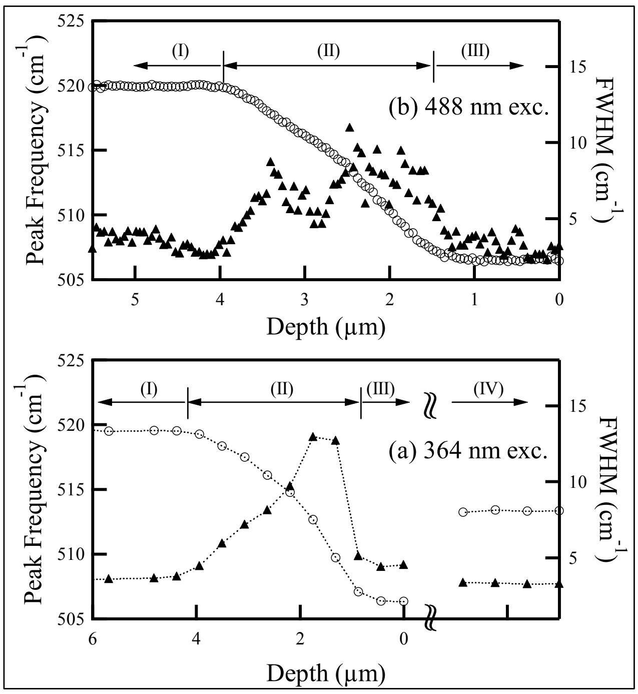

Fig. 3. Peak frequencies (○) and FWHMs (▲) of Si-Si bands of the Si and $Si_{1-x}Ge_x$ layers. (I): Si substrate, (II): graded $Si_{1-x}Ge_x$, (III): $Si_{0.8}Ge_{0.2}$ buffer layer, (IV): s-Si layer.

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 strain in the top s-Si layer can be estimated from the peak frequency of the Si band [5]. The in-plane strain of the s-Si layer was estimated to be 0.77 % from the frequency of the Si band (513.3 cm^{-1}). 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.

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