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Application of optical scatterometry to microstructure changes of $Si_{1-x}Ge_x$/Si heterostructures grown by gas source molecular beam epitaxy

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The microstructure changes of $Si_{1-x}Ge_x$/Si heterostructures grown by gas source molecular epitaxy (GSMBE) were investigated by the scatterometer with angle-resolved scattering. Experimental results show that the microstructure changes with different strain distributions in pseudomorphic layers affect the surfaces of $Si_{1-x}Ge_x$/Si heterostructures, which leads to different scattering profiles. The surfaces of heterostructures grown under different growth conditions are microrough to different degree and surface quality of epilayers has a closed connection with the growth parameters and growth modes in the heteroepitaxy.

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1. Introduction

It is well known that silicon and germanium are two of the most useful semiconductor materials. According to the Si-Ge phase diagram, the solid solution can be formed at any desired composition with an adjusted band gap. Recent advance in Si epitaxial technology has made it possible to grow pseudomorphic $Si_{1-x}Ge_x$ alloys with good crystallinity and electronic properties [1]. The addition of Ge extends the wavelength range of Si, which allows an additional degree of freedom in bandgap engineering [2, 3]. High-quality surface of $_{Si\mathit{1}}$-x$_{G}$ex epilayers and high-quality $_{Si\mathit{1}}$-x$_{G}$ex alloys are essential for the realization of device structures for planar fabrication techniques in the semiconductor

The use of light scattering to measure surface roughness has held wide interest for many years [4]. Not only has the technique been the subject of a great deal of research, but light-scattering systems have also been employed in a practical way to measure the surface quality of optical components and semiconductor applications [5-9]. For optical surfaces even a small degree of roughness produces measurable light scatteri. It was found that light scattered by microroughness has a high degree of polarization in all scattering directions [10].

For semiconductor applications light scattering has been used to map and size particulates on silicon wafers for microroughness characterization in the semiconductor industry. In fact, it is only recently that microroughness has many years [5, 6], but in contrast to the optical industry, it has only recently been seriously considered as a source of been considered a serious problem in semiconductor industry [6].

Because of the strain in $Si_{1-x}Ge_x$ epilayers, surface quality has a closed connection with the growth parameters and growth modes in the heteroepitaxy. In order to characterize microroughness of semiconductor surface and optimize the design of electronic and optoelectronic devices, an accurate knowledge of the relation between the surface microroughness and the strain distribution in these heterostructures is essential. Light scattering has been shown to be a powerful diagnostic technique for characterizing surface quality of semiconductor [7, 11, 12].

In this paper we investigate surface characterization of $Si_{1-x}Ge_x$/Si heterostructures grown by GSMBE using a scatterometer with angle-resolved scattering. The results show that surfaces of $Si_{1-x}Ge_x$/Si heterostructures have a closed connection with the microstructure changes in pseudomorphic layers.

The scattering profiles from the surfaces of $Si_{1-x}Ge_x$/Si heterostructures are different for the samples with different strain distributions, even if all samples display mirror-like surface morphology, which means that the surfaces are microrough to different degree for samples grown under different growth conditions in the heteroepitaxy.

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2. Experiments

A. Gas Source Molecular Beam Epitaxy

Growth of $Si_{1-x}Ge_x/Si$ alloys and multi-quantum wells was done in a modified MBE system by combining a gas-handling system, which had a vacuum load-lock entry and turbomolecular pump to produce pressure of about 2×10^{-4} Torr during growth [13, 14]. The growth chamber was provided with an ion pump which maintained a background vacuum 4×10^{-10} Torr. Pure Si_2H_6 and GeH_4 were selected as the source material. The substrates used for the epitaxial depositions were (001)-oriented Si wafers. Prior to the growth, the substrate temperature was raised up to 900 °C to desorb the remaining native oxide for 30 min, and the substrate temperature was brought down to the growth temperature. *In situ* Reflection High-Energy Electron Diffraction (RHEED) was used to monitor the surface crystallinity and smoothness. After all the growth, the surface of samples are mirror-smooth.

B. Scatterometer with angle-resolved scattering

The entire scatterometer assembly was constructed on a standard vibration isolated optical table, the surface of which was parallel to the plane of incidence. Stable He-Ne laser source with a polarized output 3 mW and a wavelength l = 632.8 nm was used. A slightly converging linearly polarized beam was sent toward the sample. The detection system, which consists of a photomultiplier and polarization optical elements, was mounted on a 70 cm long arm and pointed toward the sample. The arm was rotated under computer control, and the sample mount was attached to a computer-controlled rotation stage fixed to the optical table so that the angle of incidence could be easily determined and modified by rotating the sample. To reject effects due to background light in the lab, a stabilized mechanical chopper was placed in the incident beam, and detector signal was measured using a computer controlled, lock-in amplifier (Stanford Research System, SR530) synchronized with the chopper reference signal. The incident wave with an incident angle of 10° is linearly polarized in a direction orthogonal or parallel to the plane of incidence (*s* or *p* polarization, respectively) or oriented to +45° respect to the plane of incidence. The signals with a scattering angle of ± 1° around the specular direction were measured because all samples show mirror-like surface morphology. The incident beam was arbitrarily attenuated to a constant value for all the measurements. The intensity data were taken as a function of the scattering angle.

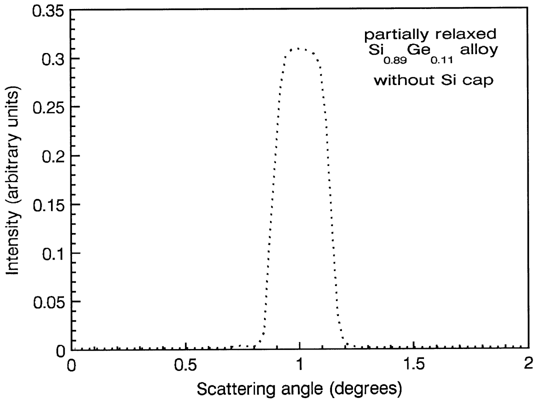

FIG. 1 Measured angular-scattering distributions for *s* → *s* polarization combination from surface of partially relaxed $Si_{0.89}Ge_{0.11}/Si(001)$ alloy without Si cap. The top of the scattering profile is nearly flat.

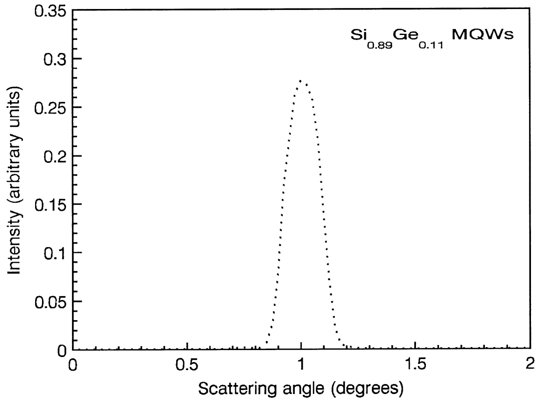

FIG. 2 Measured angular-scattering distributions for *s* → *s* polarization combination from surface of $Si_{0.89}Ge_{0.11}/Si(001)$ MQWs without Si cap. The scattering profile displays Gaussian-like profile.

3. Results and discussion.

Representative experimental results obtained from the scatterometer with angle-resolved scattering for the surfaces of $Si_{1-x}Ge_x/Si$ samples are plotted in Figs. 1 to 3, where we present only measurements taken with *s* → *s* polarization combinations. The scattering profiles are different with the samples, even if all samples display mirror-like surface morphology. For partially relaxed $Si_{0.89}Ge_{0.11}/Si$ alloy without Si cap, the top of the scattering profile is nearly flat (Fig. 1). The scattering

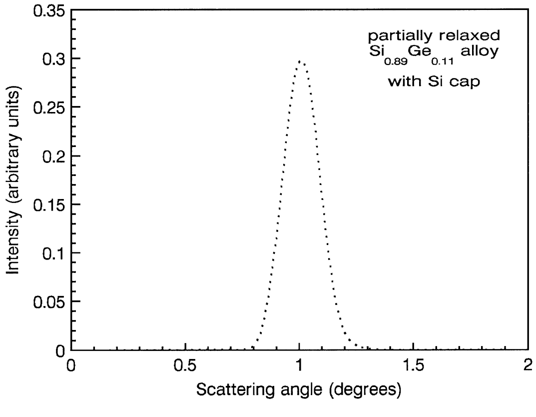

FIG. 3 Measured angular-scattering distributions for *s* → *s* polarization combination from surfaces of partially relaxed

$Si_{0.89}Ge_{0.11}$/Si(001) alloy with 10 nm Si cap. The scattering profile shows Gaussian profile.

profile of $Si_{0.89}Ge_{0.11}$/Si multi-quantum wells (MQWs), however, shows Gaussian-like profile (Fig. 2). The scattering profile of partially relaxed $Si_{0.89}Ge_{0.11}$/Si alloy with 10 nm Si cap displays Gaussian profile too (Fig. 3), which is quite different from that of partially relaxed $Si_{0.89}Ge_{0.11}$/Si alloy without Si cap (Fig. 1).

For $Si_{1-x}Ge_x$/Si MQWs, $Si_{1-x}Ge_x$ and Si alternatively co-deposit onto a Si (100) surface, which leads to the formation of strained $Si_{1-x}Ge_x$ and Si epilayers, i.e., the compressive strain within $Si_{1-x}Ge_x$ epilayer and tensile strain within Si layers. Obviously, the strain distribution of $Si_{1-x}Ge_x$/Si MQWs is different from that of partially relaxed $Si_{1-x}Ge_x$/Si alloy. Because of the tensile strain within Si layers, partially relaxed $Si_{1-x}Ge_x$/Si alloy with 10 nm Si cap (Fig. 3) shows different scattering profile from that of partially relaxed $Si_{1-x}Ge_x$/Si alloy without Si cap (Fig. 1). The microstructure changes with different strain distributions in $Si_{1-x}Ge_x$ epilayers affect the surfaces of $Si_{1-x}Ge_x$ heterostructures, which leads to different scattering profiles.

4. Conclusion

The microstructure changes of $Si_{1-x}Ge_x$ pseudomorphic layers were studied using a scatterometer with angle-resolved scattering. The signals with a scattering angle of ± 1° around the specular direction were measured. The scattering profiles are different for the samples, even if all samples display mirror-like surface morphology. For partially relaxed $Si_{0.89}Ge_{0.11}$ alloys without Si cap, the top of the scattering profile is nearly flat. The scattering profile of $Si_{0.89}Ge_{0.11}$/Si MQWs, however, shows Gaussian-like profile. The scattering profile of partially relaxed $Si_{0.89}Ge_{0.11}$ alloys with Si caps display Gaussian profile too, which is quite different from that of partially relaxed $Si_{0.89}Ge_{0.11}$ alloys without Si caps. Experimental results show that the microstructure changes with different strain distributions in $Si_{1-x}Ge_x$ epilayers affect the surfaces of $Si_{1-x}Ge_x$/Si heterostructures, which leads to different scattering profiles. The surface microroughness is related to the microstructure changes in pseudomorphic layers. The surfaces of heterostructures grown under different growth conditions are microrough to different degree and surface quality of epilayers has a closed connection with the growth parameters and growth modes in the heteroepitaxy. Optical scattering is of significance to characterize surface microroughness of epilayers.

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