Microstructure of SiGe/Si Films Studied Using High-Resolution X-ray Microdiffraction

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Introduction

Heteroepitaxial $Si_{1-x}Ge_x$/Si(001) films are of great interest and growing importance to the microelectronics industry[1] for use as substrates for high-mobility field-effect transistors. An understanding of the density and distribution of defects in these films and their effect on electronic properties is necessary for the development of future high-speed devices. Using high-angular-resolution x-ray microdiffraction (XRMD) we find that the microstructure of a *step-graded* strain-relaxed $Si_{0.83}Ge_{0.17}$ film with a low threading-dislocation density can be described by columnar "micrograins" that extend from the misfit dislocation network up to the wafer surface and have essentially uniform (001) lattice spacing. They have narrow rocking angular widths of 0.013°-0.02° and tilt angles that range from ~0.05° to 0.2° with corresponding average micrograin areas of ~2.0 to 0.8 µm^2. By contrast, rocking curves of a *uniform* strain-relaxed $Si_{0.71}Ge_{0.29}$ film with a high density of threading dislocations, although taken with the same instrumental resolution, are almost featureless, which is indicative of a much finer microstructure (smaller micrograins).

Methods and Materials

We have investigated two classes of $Si_{1-x}Ge_x$/Si structures: (1) *uniform*: uniform composition $Si_{1-x}Ge_x$ films grown directly on Si, and (2) *step-graded*: uniform composition films grown on thin, Ge-step-graded buffer layers on Si. Strain relaxation by nucleation of 60° misfit dislocations takes place by different mechanisms in the two classes. Uniform films relax initially by surface roughening followed by random nucleation of 60° misfit dislocations resulting in high densities (~10^{10} cm^{-2}) of threading dislocations at the wafer surface. Alternatively, dislocation multiplication occurs in the step-graded films, which therefore have low threading-dislocation densities (~10^5-10^7 cm^{-2}). Accordingly, one expects details of the microstructure (size of micrograins) to differ substantially in these two classes of films.

We have studied the microstructure of a step-graded, 3.0 µm $Si_{0.83}Ge_{0.17}$ film 97% relaxed (S1) and a 1.0 mm, 94% relaxed $Si_{0.71}Ge_{0.29}$ uniform film (S2). Experiments used 8.05 keV (λ=1.54 Å) photons from the x-ray undulator source of the 2-ID-D SRI-CAT end station. High angular resolution XRMD measurements were performed using a 2.5-µm-nominal-diameter pinhole. The (004) rocking curve from the Si(001) substrate had a full-width at the half-maximum (FWHM) of 0.005°.

Results and Discussions

Figures 1a and 2 show series of θ scans (rocking curves) versus sample vertical position from the two samples. All spectra from the step-graded, low threading-dislocation density sample S1 (Fig. 1) show a complex fine structure resolved to a scale of ~0.01°-0.02°. This fine structure is resolved here for the first time

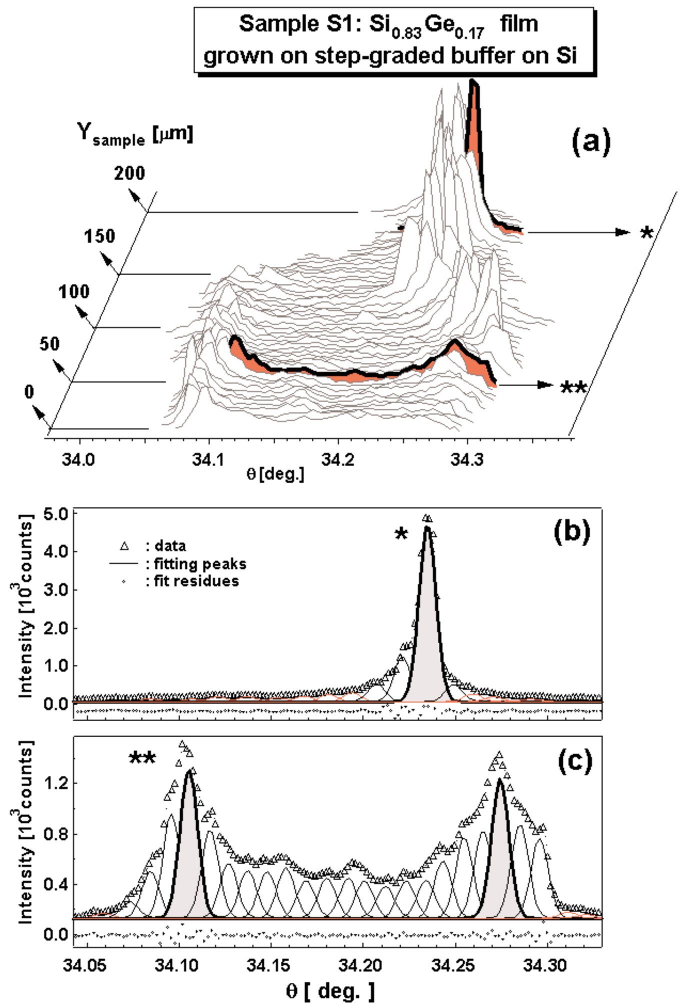

FIG. 1. High-resolution x-ray microdiffraction rocking curves from the step-graded sample S1 taken in a sequence of 4.0 µm vertical sample position steps.

due to the ~0.005° high angular resolution of the incident x-ray microbeam and is due to the local microstructure at the various illuminated spots. The data confirm that this class of films consists of multiple tilted "micrograins."[2] By contrast, rocking curves of sample S2 (Fig. 2), although taken with the same instrumental resolution, are almost featureless. This is indicative of a much finer microstructure.

For the low-dislocation-density sample S1, the high angular resolution allowed a further quantitative analysis of the rocking curves. First, we noticed that when individual, relatively isolated micrograins are seen, e.g., the highlighted gaussian in Fig. 1b, the peak width is ~0.013°. We then estimated the range of tilt angles

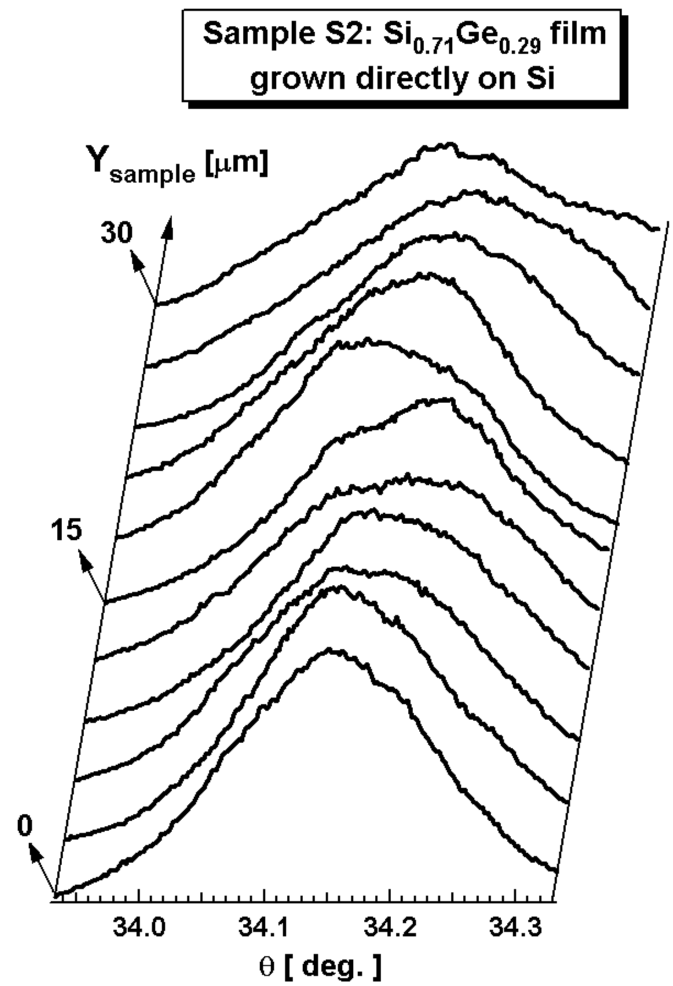

FIG. 2. High-resolution x-ray microdiffraction rocking curves from the uniform sample S2 taken in a sequence of 3.0 µm vertical sample position steps.

and density and sizes of micrograins in S1 by using a simple model where each micrograin is described by a Gaussian peak with a fixed angular width, as shown in Fig. 1b and 1c. In this model, the intensity of a micrograin is proportional to its illuminated area. We have fitted ~100 rocking curves taken at a number of positions with a total sampled area of ~10^4 mm^2 for sample S1. Using our Gaussian fitting model, we have the following general description of the microstructure for the step-graded sample S1. Sharp, tilted rectangular columnar micrograins (~0.013°-0.02° angular FWHM and ≤0.01° range of θ_B-equivalent δd/d lattice parameter variation) account for typically 80-90% of the total scattering intensity. The most prevalent θ rocking curves (~50% of a total of 250) had a medium local range of tilts angles (~0.05°-0.12°) and average micrograin size of ~1.5 µm diameter. About 15% of the rocking curves had a narrow local range of tilt angles (≤0.05°) with an average size of 2.3 µm and a maximum observed size of 4.5 µm. About 35% of the rocking curves had a wide local range of tilt angles (~0.12°-0.23°), an average grain size of 0.9 µm, and a significant number of micrograins below 0.6 µm. The shapes of the rocking curves and average tilt angles tend to correlate over distances of 10-20 µm with intermittent rapid changes in shapes and average angle.

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