Quantitative HAADF study of Ge diffusion in strained Si at atomic scale

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1. INTRODUCTION

To continuously increase microelectronics performances, simple geometry scaling of component is no longer sufficient. Different strategies have been developed to overcome this technical challenge. A first one is based on III-V alloys such as GaAs or InP, possessing attractive properties, but these materials hardly integrate the mainstream manufacturing processes based on silicon. Another approach consists in using strained Si [1], when deposited on relaxed $Si_{1-x}Ge_x$ pseudo-substrate. In this configuration, carriers mobility is highly increased and, for instance, short channel effects are limited [2,3].

This concept is now applied to low dimensional objects, such as ultrathin multilayers or nanowires to take advantage of the quantum effects. By tuning bang-gap energies, one should increase solar-cells efficiency or drastically reduce the switching delay of field effect transistors. In this context a perfect control of layers composition on short scales is required. Small fluctuations would drastically change opto-electronic properties. In this study, we focus on germanium diffusion during the growth of a strain Si layer on a relaxed $Si_{0.8}Ge_{0.2}$ substrate, by molecular beam epitaxy. A chemical analysis of the interface is performed at atomic scale, using High Angle Annular Dark Field (HAADF). Details of this work are fully described in ref. [4].

2. RESULTS

2.1 Experimental details

The sample studied was grown by Molecular Beam Epitaxy (MBE). A 20 nm thick Si layer was deposited on a relaxed $Si_{0.8}Ge_{0.2}$ virtual substrate at 450°C. To avoid any contamination, the wafer was cleaned by a modified Shiraki procedure before introduction into the MBE setup.

The specimens taken for electron microscopy observations were prepared by wedge mechanical polishing, with an angle close to 2°, both in ⟨110⟩ and ⟨100⟩ directions. Before introduction into the microscope, surfaces were cleaned with a low energy (less than 300 eV) Ar-ion beam for a short time (15 min). Micrographs were obtained on a FEI-Titan 80-300 cubed transmission electron microscope (TEM) equipped with an aberration corrector of the probe-forming lens. The microscope was operating at 200 keV, with a convergence semi-angle set to 18 mrad, leading to a probe size of about 0.1 nm. Inner-angles were 60 mrad and 30 mrad for HAADF and Low-Angle Annular Dark Field Detector (LAADF), respectively.

Finally, HAADF multislice image calculations have been carried out using the QSTEM simulation suite [5], using the experimental microscope acceleration voltage, probe-forming aperture and inner-detector angle described above. A corrected probe was employed (C3 = 4 µm, Cc=1.4 mm, and energy spread of 1.4 eV) with a defocus set to -5 nm. The sample was modeled as a bulk Si 3×3 supercell, 10.5 nm thick, observed along ⟨100⟩ zone axis. Ge impurities were introduced in the supercell, substituting Si atoms. For each simulation, thermal diffuse scattering was taken into account by averaging 30 configurations and using atomic weight to approximate displacements at 300 K.

2.2 Experimental HAADF observations

In thinnest lamella regions, one can observe intensity fluctuations of the individual atomic columns, either on the brighter $Si_{0.8}Ge_{0.2}$ substrate or on the darker Si layer (see Fig. 1). They are attributed to their local composition variation. These fluctuations disappear in thicker areas, averaged by higher atoms amount per atomic column. Moreover, a partial strain relaxation, due to the thinning procedure, leads to a darker band around the interface. It has been reproduced using finite element modeling (see Fig. 2).

Figure 1. HAADF observation of an epitaxial Si layer (dark) on $Si_{0.8}Ge_{0.2}$ substrate (bright). Atomic column intensity variations are due to chemical composition variations.

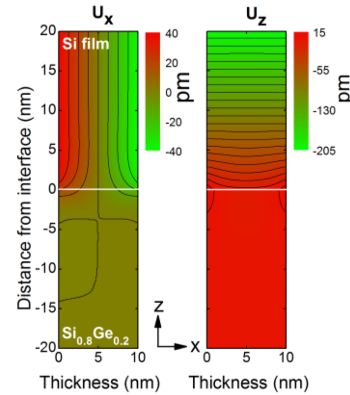

Figure 2. Finite element modeling of lamella deformation for a strained Si layer on $Si_{0.8}Ge_{0.2}$ substrate.

2.3 Quantitative intensity measurements, simulations and interpretation

Quantitative analysis of the HR-HAADF STEM micrographs was carried out, modelling each atomic column intensity as a Gaussian curve. Statistically, the column to column intensity variations were interpreted as a binomial distribution of Ge impurities. Coupled with HAADF simulations (see Fig. 3), we were finally able to determine the average atomic column composition as a function of its distance from the interface (see Fig. 4).

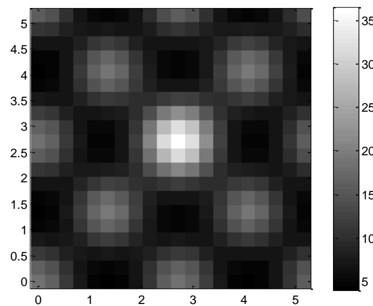

Figure 3. HAADF micrograph simulation of a Si supercell containing 3 Ge substitutional impurities.

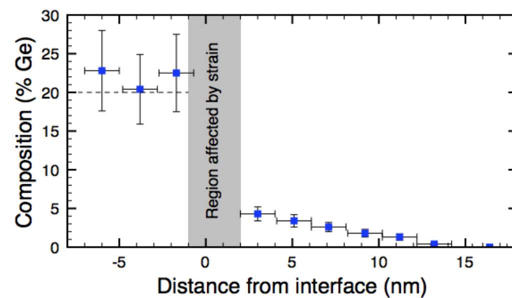

Figure 4. Ge composition profile obtained from the statistical analysis of HAADF intensities.

3. CONCLUSION

This study demonstrates the possibility of a quantitative study of sample chemical composition at atomic scale, using High Resolution HAADF measurements. Moreover, considering Si epitaxy on SiGe substrate at low temperature, a diffusion of Ge atoms up to 10 nm occurs during growth process, limiting interface sharpness.

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