Quantitative study of Ge diffusion in strained Si during epitaxial growth

G. Radtke[1], L. Favre[2]*, M. Couillard[3], G. Amiard[2], I. Berbezier[2] and G.A. Botton[4]

[1] IMPMC-CNRS UMR 7590, Université Pierre et Marie Curie-Paris 6, Campus Jussieu, 4 place Jussieu, F-75252 Paris Cedex 05, France
[2] IM2NP-UMR 7334, CNRS, Aix-Marseille Université, Faculté des Sciences de Saint-Jérôme, F-13397, Marseille, France
[3] Brockhouse Institute of Materials Research and Canadian Centre for Electron Microscopy, McMaster University, 1280 Main Street West,Hamilton, Ontario L8S 4M1, Canada
[4] Department of Materials Science and Engineering and Canadian Centre for Electron Microscopy, McMaster University, 1280 Main Street West, Hamilton, Ontario L8S 4M1, Canada
*Email: luc.favre@im2np.fr

To continuously improve microelectronics performances, strained silicon is increasingly used [1], including for low dimensional objects such as nanowires or ultra-thin films [2,3]. 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 by molecular beam epitaxy of a strain Si layer on a relaxed $Si_{0.8}Ge_{0.2}$ substrate. A chemical analysis of the interface is performed at atomic scale, using probe corrected High Angle Annular Dark Field (HAADF) microscopy. Micrograph analysis reveals intensity fluctuations of the individual atomic columns, due to their local composition variations (see fig. 1). In order to quantitatively estimate Ge diffusion into the Si layer, we preceded to an extraction of atomic columns intensities, modelling micrograph as the sum of Gaussian curves. Then we studied HAADF atomic column intensity using multislice simulations.

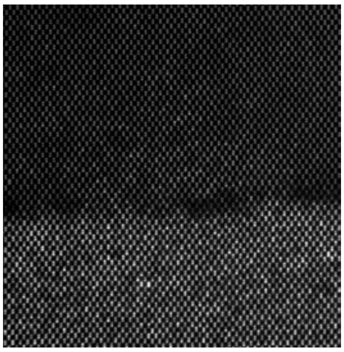

Figure 1: HAADF observation of an epitaxial Si layer (dark) on $Si_{0.8}Ge_{0.2}$ substrate (bright). Atomic column intensity variations are due to chemical composition variations.

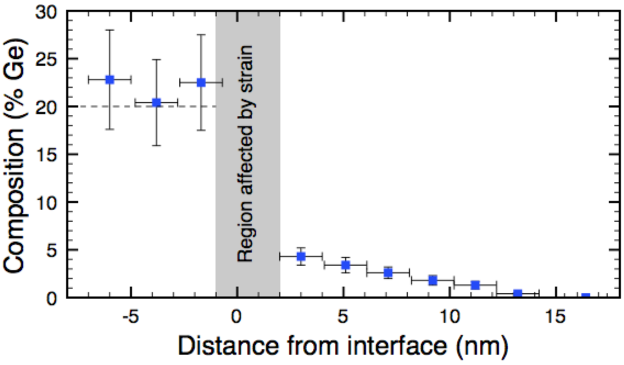

Figure 2: Ge composition profile obtained from the statistical analysis of HAADF intensities.

We demonstrated that it depends both on Ge atoms amount per column and their relative position into the column. Based on a statistical model considering the column composition as a binomial distribution, we finally determined the average atomic column composition as a function of its distance from the $Si/Si_{0.8}Ge_{0.2}$ interface: a diffusion of Ge atoms up to 10 nm occurs during growth process, limiting the $Si/Si_{0.8}Ge_{0.2}$ interface sharpness (see fig. 2). Details of this work are fully described in ref. [4].

1. K.-W. Ang et al., IEEE Electron Device Lett. 28, 609 (2007)
2. D. J. Paul, Semicond. Sci. Technol. 19, R75 (2004)
3. F. Capasso, Science 235, 172 (1987).
4. Radtke et al., Phys. Rev. B 87, 205309 (2013)