

Quantitative HAADF study of Ge diffusion in strained Si

G. Radtke¹, L. Favre^{2*}, M. Couillard³, G. Amiard², I. Berbezier² and G.A. Botton⁴

¹*IMPMC-CNRS UMR 7590, Université Pierre et Marie Curie-Paris 6, Paris, France*

²*IM2NP-UMR 7334, CNRS, Aix-Marseille Université, Marseille, France*

³*Brockhouse Institute of Materials Research and CCEM, McMaster University, Hamilton, Ontario, Canada*

⁴*Department of Materials Science and Engineering and CCEM, McMaster University, Hamilton, Ontario, Canada*

*luc.favre@im2np.fr; Phone: (+33) 4 91 28 91 59; Fax: (+33) 4 91 28 91 61

To continuously improve microelectronics performances, strained silicon is increasingly used, including for low dimensional objects such as nanowires or ultra-thin films. 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. 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. 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.