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Diffusion in Si_xGe_{1-x}/ Si Nanowire Heterostructures

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Heterostructured nanowires of IV-IV materials have attracted attention for their potential as important building blocks to construct nanoscale electronics circuits and light-emitting devices. Recently, one-dimensional SiGe/Si heterostructures have been successfully generated by the metal-catalyst VLS mechanism, self-catalyst VLS mechanism and oxide-assisted growth (OAG) mechanism [1-3]. The elevated temperatures used for the processing of SiGe/Si devices may lead to interdiffusion between these miscible components, which would degrade the functionality of the device. Diffusion mechanisms in nanostructured materials are not well understood, and fundamental studies on diffusion mechanisms and kinetics in nanowires are necessary.

We successfully grew metal-free SiGe tip / Si nanowire heterostructures by pulsed laser vaporization (PLV). This heterostructure provides a model structure for diffusions studies in the nanowire geometry. We focused on [111]-growth SiGe tip/Si nanowire heterostructures and studied Ge diffusion behavior at different annealing temperatures from 200^oC to 800^oC in N_2/H_2 atmosphere. Structural and chemical characterizations of nanowire heterostructures were carried out using transmission electron microscopy (TEM) / scanning TEM (STEM) and complementary energy-dispersive x-ray spectroscopy (EDS). A dark-field STEM image of an as-grown sample is shown in Fig. 1A. High-resolution transmission electron microscopy (HRTEM) images of as-grown sample and sample annealed at 400^oC are shown in Fig. 1B and 1C, respectively. Corresponding to the area enclosed by the box shown in Figure 1B, Fig.1D shows a coherent twin boundary in the Si nanowire. Fig.2A and Fig. 2B show Ge concentration profiles along nanowire growth direction [111] determined by quantitative analysis of energy-dispersive x-ray spectroscopy for as-grown and 400^oC annealed samples. Ge compositions in Si nanowires were quantified by the ζ factor approach [4]. The ζ factor and absorption correction considered the Si and Ge Kα lines from at standard SiGe alloy thin-film sample.

A limited-source diffusion mode was applied to determine the diffusion coefficient at different annealing temperatures from 200^oC to 800^oC. We evaluated the activation energy barrier for Ge diffusion in [111] growth Si nanowire to be 0.62eV by fitting an Arrhenius plot of the Ge diffusion coefficient. We found this activation barrier to be much lower than the value for Ge diffusion in Si bulk. In fact, the 0.62eV activation energy barrier is similar to the previous reported aviation energy barrier of 0.67eV for Ge diffusion on Si surface [5]. Proposed mechanisms for diffusion in the nanowire geometry will be discussed.

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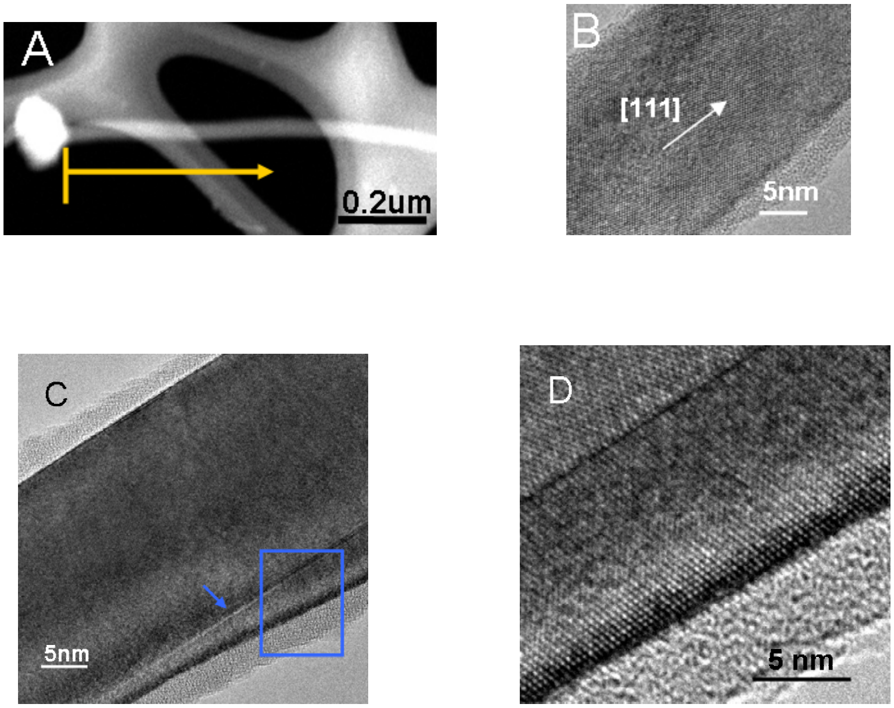

Figure 1: (A) Dark-field STEM image of a SiGe tip/ Si nanowire heterostructure grown in [111] direction. (B) High-resolution TEM image of as-grown sample. (C) High-resolution TEM image of a SiGe tip/Si nanowire heterostructure annealed at 400°C. (D) High-resolution TEM image of area corresponding to the box in (C).

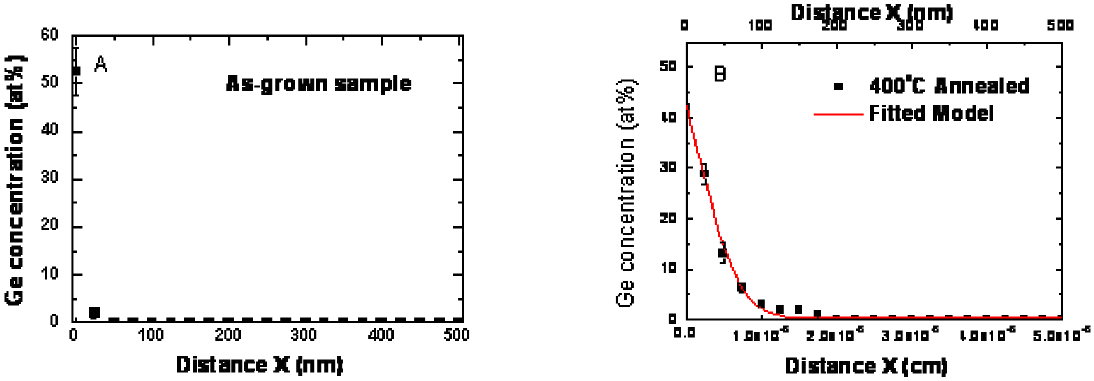

Figure 2: (A) Ge concentration profile along the line shown in Fig. 1(A) for as-grown sample. (B) Ge concentration profile for annealed sample at 400°C for 1h in N_2/H_2 (flow ratio 90:10) atmosphere. Red line is the fitted curve by the Limited-source diffusion mode.