Growth and study of self-organized Ge quantum wires on Si(111) substrates

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Self-organized Ge quantum wires were grown on regular atomic steps formed along $[\bar{1}10]$ direction on Si(111) substrates by annealing at 870 °C in vacuum. The samples were then studied by atomic force microscopy, polarization-dependent Raman scattering, and low temperature photoluminescence spectroscopy. The results suggest that good quality Ge quantum wires were formed and clear quantum confinement-induced quantization in the wires was observed. © *1999 American Institute of Physics.* [S0003-6951(99)02417-1]

Recently, low dimensional semiconductor quantum structures have attracted much attention owing to their interesting properties in quantum physics and their potential applications. In particular, self-organized nanostructures are of particular interests due to the fact that self-organization provides a possible way to realize nanostructures without process-induced defects or damage, which are frequently seen in the samples defined by e-beam lithography and reactive ion etching. Most of the published work on self-organized nanostructures was on self-organized quantum dots (QDs).[1–3] The purpose of those studies is to understand the growth mechanism of island formation and to better control their sizes and spatial distribution for device applications, such as the self-organized InAs QD based laser.[4] Although the growth mechanism is still elusive, the growth of good quality QDs with the size uniformity within ±3% has been reported[5] and the QDs can be selectively grown on predetermined surface location.[6] To date, little work has been reported on self-organized quantum wires[7] since self-organized quantum wires are much harder to be realized than self-organized QDs.

Early studies on quantum wires dated back to about a decade ago. Growth on the vicinal planes of various substrates was employed to prepare quantum wires.[8] Recently, Tersoff *et al.*[9] reported their theoretical studies and suggested that it would be possible to create atomic height steps on the vicinal planes of a semiconductor substrate as templates for the growth of quantum wires. In addition, previous research has shown that self-organized Ge QDs are somehow aligned on the upper edges of the surface kinks on tilted Si(100) substrates,[10] suggesting a possible way of forming self-organized Ge quantum wires on Si substrates as the step edges are energetically preferred by the Ge adatoms. In this work, we report the growth of self-organized Ge quantum wires on the regular atomic steps created on Si(111) substrates and our optical studies of the quantum wires. Strain effects and quantized optical transitions related to the ground states and the first excited states in the wires due to lateral potential confinement are observed.

The substrates used in this study were 0.5° miscut *p*-type Si(111). They were cleaned by a standard Si wafer cleaning procedure before Si molecular beam epitaxial (MBE) growth. The samples were grown using a gas source MBE system with a Si_2H_6 gas source and a Ge Knudsen source. After the chemical cleaning, the wafers were loaded into the ultrahigh vacuum (UHV) MBE chamber, and then heated to 870 °C to remove the surface native oxide layer. Regular atomic steps were formed with the step height of about 0.5 nm and the terrace width of about 110 nm along [110] on the surface after the annealing (see Fig. 1). After growing a 300 nm Si buffer layer, Ge was deposited at a growth temperature of 600 °C and a growth rate of about 0.01 nm/s. The Ge growth rate was stabilized by controlling the cell temperature to within an error of ±1 °C, and the rate was calibrated with Auger electron spectroscopy (AES) and atomic force microscopy (AFM) measurements. The sample morphology was then studied by AFM.

The Raman measurements were performed in backscattering configuration at room temperature on a micro-Raman system using the 514.5 nm line of an Ar^+ laser as the excitation source. Low temperature photoluminescence (PL) spectra were also obtained at 4.2 K on a standard cryostat system using the 514.5 nm laser excitation with a power density of about 3 W/cm^2. The PL signal was detected with a

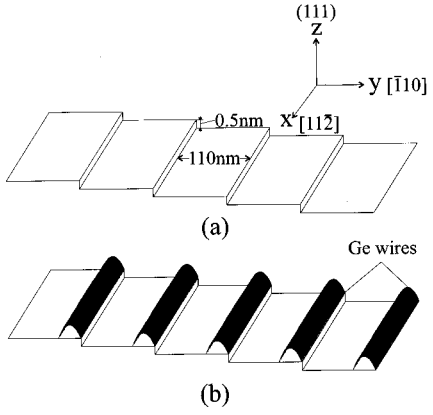

FIG. 1. Schematic diagrams of the Si(111) surface before and after the Ge growth. (a) The periodic atomic step formation along [110] direction after annealing but before the Ge growth; (b) after the growth of self-organized Ge wires along [112] direction.

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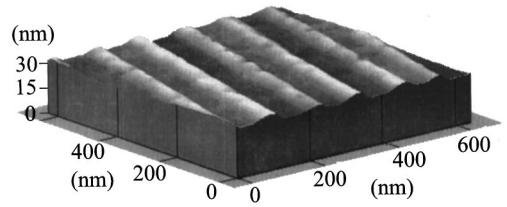

FIG. 2. Typical AFM image of self-organized Ge quantum wires on Si(111) substrate with 10 ML Ge. The most probable height and width of the wires are 4.5 and 43.4 nm, respectively.

liquid nitrogen cooled germanium detector through a 0.5 m monochromator. The slit size for the PL measurements was kept at 500 μm.

Figure 2 shows the AFM image of the self-organized Ge quantum wires on a Si(111) substrate after growing an equivalent of 10 ML (or 1.6 nm) Ge. The Ge wires are aligned along [112] direction and regularly spaced along [110] direction with the pitch size of about 110 nm. The AFM results indicated the average height of the self-organized Ge wires of about 4.5 nm and the average width of the wires of about 43.4 nm. As normally seen in the growth of Ge on Si(100), the growth of Ge on Si(111) is also Stranski–Krastanov mode growth. The former system can be monolayer and bilayer growth mode, but the latter system belongs to bilayer growth mode. Therefore, we estimated that the quantity of Ge in the wires was equivalent to about 1.1 nm, and the rest of the Ge (about 0.5 nm) should contribute to the formation of a wetting layer.

From the AFM image (Fig. 2), the Ge wires are not very smoothly distributed along the wire direction. The lateral size fluctuation of the Ge wires is believed to be caused by the wire formation mechanism: the self-organized Ge wires are the result of self-aligned self-organized Ge dots along the upper edges of the surface steps.[10] First, after the formation of regular atomic steps and the deposition of the 300 nm Si buffer layer on the Si(111) substrate, a two-dimensional (2D) Ge wetting layer forms on the surface due to the typical Stranski–Krastanov mode growth. Then self-organized Ge QDs are formed on the convex surface, which yields to the upper edge sites of the steps on the substrate. Finally, due to the energetic preference of Ge accumulation on the edge sites, more and more Ge adatoms migrate to the edge sites and fill the gaps between the self-aligned QDs along the edges, leading to the formation of self-organized Ge wires.

In order to study the properties of the Ge wires, we have performed polarization-dependent Raman scattering on the samples. Figure 3 shows the Raman spectra with the polarization of the excitation light parallel and perpendicular to the wire orientation, i.e., [112] direction. In both curves, the peak at around 520 cm^{-1} originates predominantly from the Si substrate and the Si buffer layer (Si–Si). The top curve, taken with the light polarization parallel to the wire orientation, shows a peak located at 305.1 cm^{-1}, which is attributed to the optical phonons of the Ge–Ge stretching mode. The appearance of the peak is due to the strong coupling between the excitation light and the Ge wires; while the bottom curve, with minimum light coupling to the Ge wires due to the 90° of the light polarization with respect to the orientation of the wires, the Ge–Ge mode is very weak. This result is consistent with the AFM image in Fig. 2 and confirms the existence of the self-organized Ge wires and the wire orientation.

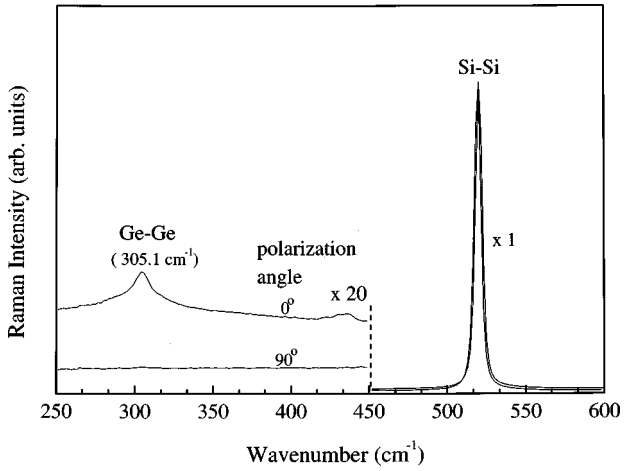

FIG. 3. Raman spectra taken from the same sample as examined in Fig. 2. The upper and lower curves are with the polarization of the excitation light parallel (0°) and perpendicular (90°) to the wire orientation, respectively. The Ge–Ge mode is seen as the incident light polarization parallel to the direction [112] of the sample. For the 90° polarization, no Ge–Ge peak was seen.

In addition, the peak of the Ge–Ge mode of the wires at 305.1 cm^{-1} is blue shifted by 3.1 cm^{-1} as compared with that from bulk Ge at 302.0 cm^{-1}, indicating a small amount of compressive strain built in the Ge wires. We do not rule out the confinement effect, which probably occurs in the wires. However, according to Sutter's study,[11] the phonon confinement effect only causes an insignificant shift of the peak to lower energy. We believe that the strain effect is dominant in our case. Assuming a negligible quantum confinement effect on the Ge Raman shift, we estimate that a blueshift of 3.1 cm^{-1} in the Ge quantum wires corresponds to an equivalent of about 0.8% lattice mismatch induced strain.[12] This is much less than the strain normally existed in a pseudomorphic Ge/Si heterostructure, which should be about 4.1% for Ge on Si surface. The partial relaxation of the compressive strain in our Ge wires confirms again the location of our Ge wires at the upper edges of the atomic height steps, which is similar to that reported by Sakamoto *et al.*,[10] who found that the Ge QDs were preferentially located on the upper edges of the kinks on the tilted Si(001) substrates and were largely relaxed.

The Ge wires located at the upper edges of the atomic surface steps should be accomplished by the distortion of the Si in the close vicinity of the Ge wires, as seen in the dry etched Si–SiGe and Si–Ge wires and dots.[13] This is further confirmed by a 4.2 K PL measurement on the same sample. As shown in Fig. 4, at the energy above 1.0 eV, the PL peaks originating from the Si region are doublets separated by 4.6 meV from each other. The weaker higher energy components of each doublet are from the strained Si regions induced by the formation of the Ge wires, suggesting the existence of a tensile strain in the Si adjacent to the Ge wires. The enhanced multiple phonon features in the PL spectrum of the Si region are also consistent with the existence of strained region in Si. The 4.6 meV blueshift of indirect band gap Si peaks corresponds to a tensile strain induced by an equivalent of about 1% lattice mismatch with respect to bulk Si. By

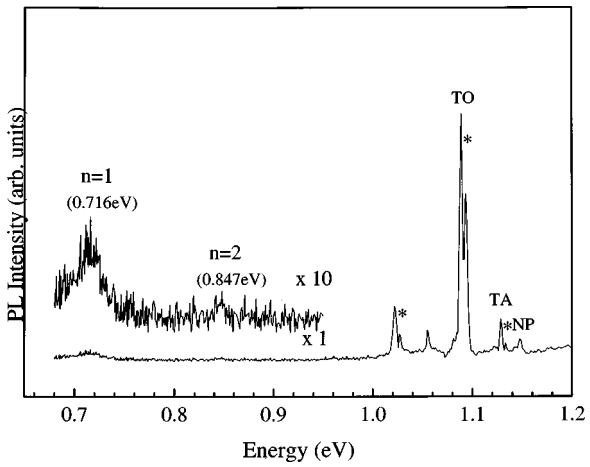

FIG. 4. 4.2 K PL spectrum of the same sample. The peaks at 0.716 and 0.847 eV are, respectively, assigned to optical transitions related to the ground and first excited states in the Ge quantum wires. The peaks are labeled as NP (1.1475 eV), TA (1.1284 eV), TO (1.0885 eV), TO+2TA (1.0545 eV), and 2TO+TA (1.0216 eV), representing the no-phonon, transverse acoustic, transverse optical, and multiple phonon modes from the Si, respectively. The separation of the doublets is about 4.5 meV.

combining results from both Raman scattering and PL results, one can conclude that a biaxial strain exists in these Ge wires grown at the upper edges of the steps.

In the PL spectrum shown in Fig. 4, there are additional two small PL peaks located at 0.716 and 0.847 eV, respectively. These two peaks are most likely from the optical transitions related to the quantized energy states in the Ge wires due to lateral wire confinement. To support this assertion, we used a simple quantum mechanics model to estimate the energies of the quantum states by assuming that the quantum wires have a lateral size of L and a height of H in the y (or [110]) and the z (or [111]) directions, respectively. Due to the fact that the lateral size L (=43.4 nm) is much larger than the height H (=4.5 nm), the quantum confinement in the y direction can be neglected. Further since the conduction band discontinuity in the z direction is very small as in a normal Si/Ge heterostructure, electron confinement in the z direction is very small as in a normal Si/Ge heterostructure, electron confinement in the z direction is neglected. Thus only the effect of heavy hole confinement is important and the optical transition energy E_n in the quantum wire is obtained by assuming an infinite barrier height on one side (air) and a limited barrier height on the other side (Si substrate), that is,

$$E_n = E_g + \Delta E_s + E_i ,$$

where E_i is determined by the equation,

$$\tan\left(\frac{\sqrt{2m^*_{h_{\mathrm{Ge}}} E_i}}{\hbar} H \right) + \sqrt{\frac{m^*_{h_{\mathrm{Si}}} E_i}{m^*_{h_{\mathrm{Ge}}} (V_0 - E_i)}} = 0,$$

where i is the quantum number related to the wire confinement along the z axis, E_g is the band gap of bulk Ge, ΔE_s is the strain induced energy shift in the Ge wires, and $m^*_{h_{\mathrm{Ge}}}$ is the effective mass of the heavy hole in Ge wires. We used $E_g = 0.718$ eV as measured by 4.2 K PL from a bulk Ge sample, and the effective mass of the heavy hole is $m^*_{h_{\mathrm{Ge}}} = 0.32 m_0$.[14] Considering that there may still be an effect of quantum confinement on the Raman peak shift, we believe that the strain data, an equivalent of 1% lattice mismatch, as extracted from the PL data may be more reliable than that from Raman analysis. The energy shift in the Ge wires induced by a biaxial strain of equivalent to 1% lattice mismatch is estimated to be about $\Delta E_s = -44$ meV.[15] By using the experimentally measured wire height (4.5 nm), and a valence band discontinuity of 0.4 eV, we can estimate that due to the Ge wire confinement in the z direction, the transition energies should be at 0.722 and 0.861 eV, respectively, with the energy separation of 139 meV. Considering some uncertainty in the effective mass and possible errors of the measurement wire sizes, this estimated number is in very good agreement with the measured data.

In summary, we have grown self-organized Ge quantum wires on Si(111) substrates by forming regular atomic steps first followed by Ge deposition. Optical studies of the Ge wires suggest that these wires have a built-in biaxial strain equivalent to about 1% lattice mismatch. In addition, quantized optical transitions due to the confinement in Ge wire were also observed. Studies are under way to improve further the understanding of the growth mechanisms and the potential applications of these structures.

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