Selectively grown GaAs nanodisks on Si(100) by molecular beam epitaxy

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III-V compounds epitaxially grown on Si have attracted a great deal of interest due to its applications in integration of optoelectronic devices with Si-based mature microelectronic technology. However, heteroepitaxy of III-V on Si generally requires time-consuming, complex thermal cycle annealing processes or micron-thick buffer layers to overcome the lattice constant and thermal expansion mismatch, and antiphase domain disorder related issues. These processes increase the material and time cost. Selective area epitaxy (SAE) on nanoscale patterned substrate has emerged as a promising technique for the growth of lattice-mismatched III-V on Si. With this approach, stress is laterally relaxed through the facet formation and side walls, leading to nearly defect-free nanostructures.

In this study, we report the growth of GaAs nanostructures on Si(100) by selective area epitaxy. In our growth scheme, SAE was applied on SiO₂ masked Si(100) nano-pattern substrates and GaAs were grown by molecular beam epitaxy (MBE). Rectangular shaped GaAs nanodisks were formed with superior material quality due to strain relaxation through facets and lateral overgrowth atop the SiO₂ mask.

It is found that a growth temperature of ~630°C yields the best selectivity and crystal quality. Figure 1 displays scanning electron microscopy (SEM) images showing a time evolution study for the growth of GaAs on Si(100). In other words, the evolution of the morphology at 630°C as a function of deposition time on Si(100) a) 30 mins, b) 60 mins, c) 90 mins, and d) 120 mins has been presented here. As can be seen, the growth initiates from one particular nucleation site, i.e. mostly on the edge of SiO₂ and then expand to fill the complete hole region to form the nanodisk arrays. As deposition proceeds, these nucleated GaAs crystals incorporate more material and expand both vertically and laterally to fill the patterned holes. Each individual nanodisk, as shown in Fig. 1(d), has lateral dimensions of ~1 μ m as it fully covers the patterned area. It is also identified from the SEM image that these disks have evident facets. The vertical side walls (4 edges of the rectangle from top view) are 4 {011} planes. The top four facets are other {011} planes. These facets indicate single crystalline nature of the growth and they are associated with the lowest total surface energy in equilibrium. Higher index facets are also present. However they are not as evident as the dominant {011} facets.

The structure of the as-grown crystal is further investigated by high resolution cross-section transmission electron microscopy (XTEM). Fig. 2(a) shows a typical XTEM image at the GaAs/Si interface. It is clearly seen that the GaAs epi-layer on Si demonstrates a pure zincblende crystal structure with an atomically sharp GaAs/Si interface, as shown in Fig. 2(c) and (d). Very few stacking faults are observed, as shown in Fig. 2(b), and they are mostly restrained at the edge of the patterned holes. These stacking faults occur when the nucleated GaAs crystal expands to reach the SiO₂ mask as they are possibly one way to release the strain energy. It is noticeable that the GaAs laterally overgrown on SiO₂ demonstrates superior quality with nearly defect-free characteristic. In fact, this lateral overgrowth mechanism has been widely utilized in III-V semiconductor systems to suppress the propagation of threading dislocations. With the reduced defect density achieved by nanoscale patterning and lateral overgrowth, these nanodisk arrays have a great potential for electronic and optoelectronic device applications.

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Fig. 1 Time evolution study of GaAs nanodisks grown on Si(100)



Fig. 2 XTEM image of (a) GaAs/Si interface; (b) GaAs laterally overgrown on top of SiO₂ showing very few stacking faults (c) left edge, (d) right edge of GaAs/SiO₂ interface showing defect free nature beyond the edge, (e) GaAs-Si covalent bond diagram