Selective epitaxial growth of Ge/Si$_{0.15}$Ge$_{0.85}$ quantum wells on Si substrate using reduced pressure chemical vapor deposition

Shen Ren (任申),$^a$ Yiwen Rong (戎亦文),$^b$ Theodore I. Kamins, James S. Harris, and David A. B. Miller

Department of Electrical Engineering, Stanford University, Stanford, California 94305, USA

(Received 22 January 2011; accepted 17 March 2011; published online 13 April 2011)

We investigate the selective epitaxial growth of Ge/Si$_{0.15}$Ge$_{0.85}$ quantum wells on prepatterned silicon substrates by reduced pressure chemical vapor deposition. A vertical p-i-n Si$_{0.1}$Ge$_{0.9}$ diode with Ge/Si$_{0.15}$Ge$_{0.85}$ quantum wells in the intrinsic region is selectively grown in holes in a SiO$_2$ mask. We find perfect growth selectivity and very low dependence on size or arrangement of the mask holes. The fabricated p-i-n diode shows very low reverse leakage current and high breakdown voltage, suggesting good epitaxy quality. The quantum-confined Stark effect in this quantum-well system is observed for wavelengths >1.5 μm at room temperature. © 2011 American Institute of Physics. [doi:10.1063/1.3574912]

Silicon-compatible photonics has attracted great research interest recently. One of its many applications is short distance optical interconnect systems. In such systems, either a direct-modulated laser source or an optical modulator is needed to transform the electrical signal into an optical signal. Although there have been many attempts to realize a Si-compatible light source, practical implementation remains challenging for the near future. On the other hand, Si-compatible optical modulators, either electrorefractive or electroabsorptive, have been demonstrated. In 2005, Kuo et al. demonstrated the quantum-confined Stark effect (QCSE) in germanium quantum-well structures. By changing the applied electrical field across the quantum wells, the absorption coefficient of the structure can be significantly modified, hence realizing electrical-to-optical conversion. This opens an approach to realizing efficient, CMOS-compatible optical modulation. Indeed, several devices based on this physical mechanism have already been demonstrated, showing large bandwidth, low drive voltage, and high-speed operation.

However, most of the work to date in this quantum-well material system used bulk epitaxy on unpatterned Si substrates. For greater integration flexibility and better process control, selective epitaxial growth is highly desirable. On the other hand, there has been much work on selective epitaxial growth of bulk Ge for nanoelectronic applications, as well as for photonic applications. Selective epitaxy is crucial to integrating Ge/SiGe quantum-well structures monolithically with silicon-on-insulator waveguides, or with other (e.g., electronic) devices. It also enables the integration of several different epitaxy designs simultaneously on the same substrate through multiple selective epitaxial growth steps. In this letter, we investigate the selective epitaxial growth of Ge/Si$_{0.15}$Ge$_{0.85}$ quantum wells on patterned Si substrates using reduced pressure chemical vapor deposition (RP-CVD).

We start with a 100-nm-diameter, (100)-oriented silicon substrate lightly doped with boron (10–20 Ω cm), and thermally grow a 1.5 μm thick SiO$_2$ layer at 1100 °C. Part of this oxide will act as the growth mask for later epitaxial growth. Various windows with different widths along the [110] direction are patterned using I-line optical lithography. Reactive ion etching is used to etch the majority of the oxide thickness (1.45 μm). Then a 20:1 buffered-oxide wet etch is used to remove the remaining 50 nm oxide in the growth window. The combination of dry etch and wet etch helps to avoid any potential plasma damage to the underlying crystalline Si in the growth window and is crucial for the quality of the subsequent epitaxial materials. The patterned substrate then goes through an “hydrofluoric acid (HF)-last” RCA clean, and is immediately loaded into an Applied Material Centura™ RP-CVD system. After a 1000 °C in situ hydrogen (H$_2$) bake for 5 min, a 20 nm Si seed layer is grown using dichlorosilane. After that, a vertical p-i-n diode structure is grown. Germane, silane, arsine, and diborane are used as the reactant and dopant gases with H$_2$ as the carrier gas. The growth for the entire structure is carried out at 395 °C in the surface reaction limited regime. Three 20 min in situ anneals at 850 °C are inserted in between the first 400 nm deposition to relax the grown epitaxy, and reduce the surface roughness and threading dislocation density. A schematic of the grown structure is illustrated in Fig. 1(a). The p- and the n-regions are Si$_{0.1}$Ge$_{0.9}$, doped with boron and arsenic, respectively. The i-region is 540 nm thick, which consists of ten pairs of 12 nm Ge quantum wells with 20 nm Si$_{0.15}$Ge$_{0.85}$ barriers sandwiched between two 100 nm intrinsic Si$_{0.1}$Ge$_{0.9}$ spacer layers. For quantum-well structures, the thicknesses of each layer, especially those of the quantum wells and the barriers, determine the wavelength of operation for the QCSE modulator, and hence are of critical importance.

After the growth, cross-sectional scanning electron microscopy (X-SEM) is used to investigate the selectivity, film thickness, and faceting of the epitaxy. As shown in Fig. 1(b), a planar heterostructure with very sharp boundaries between the Ge quantum wells and the Si$_{0.15}$Ge$_{0.85}$ barriers is grown at locations away from the growth window boundary. The total thickness of the epitaxial layer is 1.15 μm. Faceted growth occurs in the growth window next to the oxide mask,
The growth holes in the mask. Adatoms of the reactant species can diffuse from the masked area into the growth window, resulting in different growth rates for different growth window sizes (i.e., the “local loading effect”). Figures 2(a)–2(d) examines the epitaxy grown in trenches of various widths. The flat regions of the grown epitaxy in wide trenches are of the same thickness within SEM measurement accuracy. Moreover, the two faceted regions at the boundaries are of the same width and have the same angle with respect to the substrate independent of trench width beyond 2 μm. For trenches that are narrower than 1 μm, the two faceted regions join at the top, and the grown film is thinner. We also investigated the thickness dependence of the grown film on the mask coverage percentage (not shown in Fig. 2). In this case, the window size is kept constant while the mask width between adjacent growth windows is varied from very large to 450 nm. Again, the grown film thickness does not depend on the mask coverage percentage within the measurement accuracy. In other words, under our growth conditions, the selective growth shows no observable loading effect.

We fabricated vertical p-i-n mesa diodes out of the selective epitaxy using optical lithography, reactive ion etching, metal deposition, and liftoff. The schematic of the fabricated diode is shown in Fig. 3(a). Figure 3(b) is the current-voltage characteristic under dark conditions for a 150 × 150 μm^2 square mesa diode fabricated from a 200 × 200 μm^2 square growth window. Compared to diodes fabricated from bulk epitaxy, the diodes constructed from selective epitaxy show lower reverse leakage current (2.2 mA/cm^2 at −1 V, at least 20 times lower than diodes from our bulk epitaxy under similar conditions) and higher breakdown voltage. This suggests that the selective epitaxy has a lower threading dislocation density, and hence better epitaxial quality than nonpatterned material. We also measured the photocurrent spectra of the diode under different bias voltages, as shown in Fig. 3(c). Laser illumination from a tunable laser source is incident from the top surface of the diode. The photocurrent of the device is collected by a pre-amplifier, and measured by a lock-in amplifier. Large changes in the photocurrent spectrum are observed, corresponding to the well-known QCSE changes in optical absorption. Very sharp exciton peaks can be identified in the spectra, indicating minimal inhomogeneous broadening caused by nonuniformities of the grown quantum-well thickness. This is yet further evidence of the uniformity and quality of the selective epitaxy. Furthermore, because we are able to apply to up to 8 V dc bias (corresponding to approxi-

**FIG. 1.** (Color online) (a) Schematic cross-sectional view of the selective epitaxy on patterned substrate (not to scale). (b) X-SEM image of the grown film away from the growth window boundary. The vertical stripes are artifacts from cleavage, not intrinsic to the grown sample. Scale bar: 500 nm. (c) X-SEM image of the grown film at the growth window boundary. Scale bar: 500 nm.

as shown in Fig. 1(c). The faceted region extends about 700 nm from the mask edge, and its surface appears to be approximately a ⟨111⟩ crystal plane. No nucleation occurs on top of the oxide mask, as indicated in Fig. 1(c). Optical microscope inspection also confirms that no deposition takes place on the mask, demonstrating prefect selectivity between the growth window and the oxide mask. Furthermore, just away from the faceted region, planar quantum-well structures, of the same thickness as in the region far away from the boundary, are grown.

For selective growth, an important consideration is the sensitivity of the growth to the size, shape, and spacing of the growth window and the oxide mask. Furthermore, just to apply to up to 8 V dc bias (corresponding to approxi-

**FIG. 2.** X-SEM images of the grown selective epitaxy in various window sizes: (a) 10 μm, scale bar: 2 μm; (b) 5 μm, scale bar: 2 μm; (c) 2 μm, scale bar: 1 μm; (d) 1 μm, scale bar: 500 nm.
approximately 20 V/μm, about twice the electric field magnitude across the quantum wells as previously achieved by us in diodes from bulk epitaxy), the absorption edge is shifted into the telecommunication C-band (1530–1565 nm) without heating above room temperature in the Ge quantum-well materials system. This makes it possible to make a C-band, room-temperature, QCSE optical modulator with Ge quantum wells on Si.

In conclusion, we investigated the selective epitaxial growth of Ge/SiGe quantum-well structures on a Si substrate. Perfect selectivity and very low loading effect are achieved. Fabricated p-i-n diodes show very low reverse leakage and high breakdown voltage. With a 8.0 V dc bias, the device can operate in C-band at room temperature. This selective epitaxial growth technique will lead to more flexibility and better process control for integrating Ge/SiGe quantum well optical modulators with electronic and other photonic devices.

This work was supported in part by Oracle under Contract No. HR0011-08-9-0001 between the Government and Oracle. The views, opinions, and/or findings contained in this letter are those of the authors and should not be interpreted as representing the official views or policies, either expressed or implied, of the Defense Advanced Research Projects Agency or the Department of Defense. Shen Ren acknowledges the generous support of a Stanford Graduate Fellowship. Part of this work was performed at the Stanford Nanofabrication Facility (a member of the National Nanotechnology Infrastructure Network). We also want to acknowledge the technical support and assistance from ASML.

FIG. 3. (Color online) (a) Schematic cross-sectional view of the diode fabricated from the selective epitaxy. (b) Dark current-voltage characteristic for a 150×150 μm² square mesa diode fabricated from a 200×200 μm² growth window opening. (c) Photocurrent spectra of the same diode under different bias voltages.