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SILICON PHOTONICS

A self-assembled microbonded germanium/silicon heterojunction photodiode for 25 Gb/s high-speed optical interconnects

Received
29 July 2013Accepted
29 October 2013Published
15 November 2013Chih-Kuo Tseng¹, Wei-Ting Chen¹, Ku-Hung Chen¹, Han-Din Liu³, Yimin Kang³, Neil Na^{1,2}
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A novel technique using surface tension to locally bond germanium (Ge) on silicon (Si) is presented for fabricating high performance Ge/Si photodiodes. Surface tension is a cohesive force among liquid molecules that tends to bring contiguous objects in contact to maintain a minimum surface energy. We take advantage of this phenomenon to fabricate a heterojunction optoelectronic device where the lattice constants of joined semiconductors are different. A high-speed Ge/Si heterojunction waveguide photodiode is presented by microbonding a beam-shaped Ge, first grown by rapid-melt-growth (RMG) method, on top of a Si waveguide via surface tension. Excellent device performances such as an operating bandwidth of 17 GHz and a responsivity of 0.66 and 0.70 A/W at the reverse bias of -4 and -6 V, respectively, are demonstrated. This technique can be simply implemented via modern complementary metal-oxide-semiconductor (CMOS) fabrication technologies for integrating Ge on Si devices.

Germanium is an attractive semiconductor utilized in many of the state-of-the-art electronic and optoelectronic devices. The hole mobility of Ge which is about 4 times greater than that of Si, which makes Ge an ideal candidate for fabricating high-speed electronics devices operated beyond 100 GHz¹. In addition, the ability of monolithically integrating Ge with Si using CMOS processes allows active photonic devices such as photodetectors^{2,3}, modulators^{4,5} and light emitters^{6–8}, possibly integrated with Si-based electronic devices. However, direct heterogeneous epitaxial growth^{9–17} of Ge on Si is difficult due to the large lattice mismatch (4.2%) between Si and Ge, despite the fact that Ge BiCMOS HBTs and Ge photodetectors have been developed with good performance using this epitaxy growth approach. Alternatively, the Ge/Si integration can be achieved using wafer or die bonding of Ge on Si wafer^{18–20}. However, removing the bonded Ge substrate raises a cost issue, and meanwhile, surface flatness is a great concern of strongly affecting the bonding yield. The growth of Ge on an insulator substrate using RMG^{21–23} was previously reported as a promising method for integration of high quality Ge devices with CMOS integrated circuits (ICs). Via this technology, a RMG Ge avalanche photodetector on insulator has been demonstrated with a high operation bandwidth^{24–26}. Nevertheless, the high-level dark current caused by metal-semiconductor-metal (MSM) junctions significantly degrades the device sensitivity. In general, a Ge/Si heterojunction photodiode is preferred to have a low dark current due to the larger bandgap at the Si side. Moreover, it is easy to activate a highly doped Si for reducing series resistance, which is vital for high-speed operation of a photodiode.

In this paper, a high-performance Ge/Si heterojunction photodiode in a vertical p-i-n configuration is implemented by using a novel approach that takes advantage of surface tension to form a RMG Ge beam self-aligned and bonded onto a Si waveguide. The waveguide photodiode shows superior performances such as low dark current, high rectifying behavior, large photo-responsivity, and large operation bandwidth. More significantly, this approach may be applicable to other material systems such as GaAs and GaSb²⁷ III-V compound semiconductors and thus opens up new opportunity for making various hybrid heterojunctions on Si.

Figure 1 | Rapid melt growth (RMG) of Ge. (a) and (b) Schematics of phase transition of a Ge beam (side view) before and during rapid thermal annealing. The melting Ge solidifies and re-crystallizes from the Si seed window toward the end. All of the threading dislocation defects are confined near the seed window. (c) Micro-Raman spectroscopy of Ge before and after annealing. The Raman shift indicates that the phase changes from an amorphous state to a crystalline state. (d) High-resolution transmission electron microscopy image of RMG Ge. Clear phase contrast is observed throughout the Ge beam, revealing a single crystalline phase with low defects. (e) Selective area diffraction patterns of Ge and Si. The crystal orientations of Ge and Si are equivalent.

Results

Single-crystal, low-defect Ge beams fabricated by rapid-melt-growth method. First, an amorphous Ge (a-Ge) thin film is deposited and then patterned in a straight beam structure where the beam width is 2 μm and the length is 15 μm . These Ge beams are separated from the Si substrate by a SiO₂ layer except for the seed windows, where the Ge beam is in direct contact with Si surface. After deposition of thick cap oxide, rapid thermal annealing (RTA) is applied to make a-Ge melting and then re-crystallizing during a cooling process, occurring from the seed window toward the end of the Ge beam as illustrated in Figure 1a and 1b. The threading dislocations are confined near the seed window without proliferating to the top lateral beam structure. A more detailed description of the RMG process can be found in the method section. The annealing temperature is 950°C for 4 seconds, which is similar to the condition of source-drain activation in CMOS fabrication process. Figure 1c shows the Raman spectroscopy of the Ge thin film before and after the RMG process. The Raman shift and full width at half maximum (FWHM) of the as-deposited Ge are 270 and 42 cm^{-1} , respectively. After RTA, the Raman shift and FWHM are changed to be 299 and 4 cm^{-1} , which are very close to the values reported for a primitive Ge substrate (298 and 3.2 cm^{-1})²⁸. The high-resolution transmission electron microscopy (HRTEM) image in Figure 1d shows a monocrystalline phase of Ge. The crystal orientation of Ge atoms matches well with that of Si atoms in the substrate, according to the measured selected area diffraction (SAD) patterns displayed in Figure 1(e). It indicates that the lateral epitaxy of Ge takes places from the Si seed window and progresses toward the terminal of the Ge beam.

Self-assembled microbonded Ge on Si by surface tension. Although RMG is an effective way for producing single-crystal Ge beams, direct contact between Ge and Si forming a heterojunction is prohibited because the Ge structure should be isolated from Si by a dielectric layer (except for the seed window) during the re-crystallization process. Here we propose a Ge/Si heterojunction can be created by selectively removing the dielectric layer in a wet

etching solution after RMG and using surface tension to bring Ge and Si contact together. Figure 2 schematically illustrates the procedure. First, a RMG Ge beam enclosed by SiO₂ is immersed in a hydrofluoric acid solution for etching the oxide layer away. The Ge beam thereby is released as a cantilever in solution with one end anchored at the seed window on the substrate. Next, as the wafer is pulled out of the etchant, due to the hydrophobic nature of the wafer surface, the trapped liquid underneath the Ge cantilever beam is expelled and brings the Ge beam to the Si substrate due to surface tension. This is similar to the result of wafer or die bonding processes except being executed in microscale. Since the Ge beam is anchored on the substrate, it is not flushed away and the position is not altered after adhesion. In addition, the hydrophobic surface of Si makes no water molecules trapped at the Ge/Si contact interface. Although the Ge beam is bonded on the Si surface, the Ge/Si contact majorly relies on the van der Waals' force. To enhance the bonding strength, the device is post annealed at a temperature of 400°C for 1 hour in vacuum ambient.

The occurrence of adhesion, as the Ge cantilever beam leaves from the solution, is dependent on the dimensions of the beam structure, Young's modulus of Ge, gap height and surface energy of liquid trapped in the gap. A criterion to determine a critical cantilever beam length for adhesion is given by²⁹

$$L > \sqrt{\frac{3Et^3h^2}{8\gamma_s}} \quad (1)$$

where E is Young's modulus of Ge, t is the beam thickness, L is the beam length, h is the gap height between the beam and substrate, and γ_s is the surface energy of liquid. All these parameters are schematically described in Figure 3. For a Ge cantilever beam with a thickness of 0.3 μm and separated from the Si substrate by 50 nm, the beam length at least should be longer than 2 μm . Otherwise, the mechanical restoring force of the Ge cantilever beam can overcome the surface tension, leaving the beam standing above the Si surface without adhesion.

Figure 2 | Self-assembly of Ge beams on Si surface. (a) Step I: the wafer is immersed in a solution-based buffered oxide etchant. The Ge beams are released by etching away the enclosed cap oxide. (b) Step II: the wafer is taken out from the solution. The released Ge beams adhere to the Si surface by surface tension.

Ge/Si heterojunction photodiodes. Figure 4a depicts the configuration of the Ge/Si heterojunction waveguide photodetector. Optical wave propagating in the Si waveguide is evanescently coupled to the Ge absorber for converting optical power to photocurrent collected by the p-Ge/i-Ge/n-Si photodiode shown in Figure 4b. The detailed procedures of device fabrication can be found in the method section. Scanning electron microscopy (SEM) image of the fabricated device is shown in Figure 4c, where the Ge beam is precisely aligned to the center of the Si waveguide. In Figure 4d, the HRTEM image reveals that the crystal orientations of Si and Ge atoms match well. In between the Ge beam and Si waveguide, a thin interfacial layer emerges, which is believed to be formed during the post annealing process. This layer is estimated to be 7 nm in thickness and is

Figure 3 | Schematic of a Ge beam (side view) adhering to a Si substrate.

composed of Si, Ge and O atoms, where oxygen accounts for 30% and the others are Si and Ge by investigating the material content via in-situ energy dispersive spectrometer (EDS) system.

Electrical characteristics of devices. Figure 5 shows I-V characteristics of the self-assembled microbonded Ge/Si heterojunction photodiode with a microbonded Ge thickness of 0.7 μm . A low dark current smaller than 7 nA is observed at a reversed bias voltage of -2 V, corresponding to a dark current density of 23 mA/cm^2 . On the other hand, the forward bias current is about 5 mA at 2.5 V. These values are comparable to those of the reported Ge/Si heterojunction waveguide photodetectors fabricated by hetero-epitaxial growth^{13,16}. Photocurrent starts to saturate as the reverse bias voltage is larger than -1.2 V, suggesting the intrinsic Ge layer is completely depleted beyond this voltage. This interfacial layer between Ge and Si could be possible to introduce trap states. In order to understand the electrical property of the interfacial layer, a temperature-dependent dark current measurement is performed from 260 K to 300 K at different bias voltages. Here we analyze the origin of dark currents by using the following formula³⁰

$$I_{\text{Dark}} = BT^{3/2} e^{-E_a/kT} (e^{eV_a/2kT} - 1) \quad (2)$$

where B is a proportionality constant, T is the temperature, E_a is the activation energy, and V_a is the bias voltage. By fitting the logarithm of measured dark currents $\ln(I_{\text{dark}}/T^{3/2})$ as a linear function of $1/kT$, the activation energy can be extracted with respect to bias electrical fields shown in Figure 6. The activation energy decreases from 0.37 eV at 30 kV/cm to 0.19 eV at 92.3 kV/cm. Note that the activation energy 0.37 eV at a low bias condition is nearly half of the Ge bandgap, indicating that the Schockey-Read-Hall (SRH) recombination/generation via deep levels of trap states is responsible for the dark current. These trap states are believed to be localized near the interfacial layer. With a stronger electric field, the activation energy reduces whereas the dark current increases. This can be explained by the effective Ge bandgap narrowing resulting from large band bending, which facilitates electrons and holes tunneling through

Figure 4 | A self-assembled microbonded Ge/Si heterojunction photodiode. (a) Schematic of the device structure. The Ge optical absorber is bonded on the Si waveguide to form a vertical Ge/Si p-i-n photodiode. (b) Schematic of the device cross section. The Ge is p-type doped and the Si is n-type doped. (c) SEM of the fabricated device. The bonded 0.3 μm thick Ge beam is precisely aligned to the center of the Si waveguide. (d) HRTEM near the bonding interface. Crystal phase contrasts of Ge and Si are clearly observed and show the crystal orientations are well matched. A 7-nm interfacial layer exhibits between the Ge and Si.

Figure 5 | I-V characteristics of a self-assembled microbonded Ge/Si heterojunction photodiode. The red and black curves are the photocurrent and dark current, respectively. The bonded area and thickness of the Ge beam are $15 \times 2 \mu\text{m}^2$ and $0.7 \mu\text{m}$. The dark current is 7 nA at -2 V , corresponding to a current density of 23 mA/cm^2 . The laser wavelength is 1310 nm .

the trap states. We emphasize that from the measured I-V curves, the dark current is rather small in all biasing conditions, implying a low trap state density even in the presence of the interfacial layer.

Optical characteristics of devices. The attenuation length ($1/e$ intensity decay) of a guided wave propagating in the Ge/Si waveguide photodiode is estimated to be less than $5 \mu\text{m}$, according to a 2D finite-difference-time-domain (FDTD) simulation carried out at 1310 nm wavelength. The Ge beam length of this device is designed to be $15 \mu\text{m}$ for complete absorption. The waveguide insertion loss, including both fiber coupling loss, taper loss and waveguide propagation loss, is calibrated to be $19 \text{ dB} \pm 0.5 \text{ dB}$ via measuring 15 straight silicon waveguides with the same dimension but without Ge photodiodes on the same chip. The setup of optical measurement is described in the method section. The large waveguide propagation loss is mainly due to the rough sidewall surface of Si rib waveguides created by dry etching. By

excluding the optical insertion loss, the device responsivity is estimated to be 0.66 and 0.70 (A/W) at the reverse bias of -4 V and -6 V , respectively. The detailed characterization of photoresponsivity is displayed in Figure 7. Metal-induced absorption and scattering losses are mainly responsible for the lightly reduced responsivity, which can be improved by optimizing the Ge contact design³¹. The red curve in Figure 7 represents the measured device capacitance with respect to the bias voltage. The capacitance is generally less than 15 fF and decreases slightly with a larger reverse bias, indicating the Ge layer is completely depleted with a small junction capacitance.

Bandwidth measurement of the devices. High-frequency optical signal from an external modulator is coupled to the Si rib waveguide for measuring the device operation bandwidth (see the method section). Figure 8 displays the measured 3 dB bandwidth ranging from 12 GHz to 17 GHz , slightly increasing with the bias voltage from -4 V to -6 V . Assuming the hole saturation velocity of Ge is $6 \times 10^6 \text{ cm/s}$, the carrier transit time is thereby estimated to be 11.6 ps . On the other hand, the device RC delay time based on the measured junction capacitance and series resistance is calculated to be 7.7 ps . By considering both time constants, the analytically calculated device operation bandwidth is 17 GHz , agreeing well with the measured 3 dB bandwidth. Such an operation bandwidth is sufficient for a 25 Gb/s optical receiver application.

Discussion

A Ge/Si heterojunction waveguide photodiode is realized by exploiting surface tension to self-assemble Ge beam locally bonded onto Si waveguides. The Ge cantilever beam, fabricated by RMG method, exhibits a monocrystalline phase with the crystal orientation replicated from the Si seed window. After wet releasing, the Ge cantilever beam is precisely positioned on the top of the Si waveguide as the wafer is pulled out from the liquid surface. The bonding surfaces are hydrophobic, passivated by hydrogen atoms with less hydroxyl groups. To enhance the bonding strength, a post annealing process in vacuum is applied but introduces a thin interfacial layer in between the Ge/Si interface. While this interfacial layer may generate trap states near the heterojunction, from the measured I-V characteristics of the fabricated device, the low leaky current indicates a low trap state density and has no apparent impact on the device operation. Additionally, the I-V curve (dark current) was measured back and

Figure 6 | Measurement of temperature-dependent dark current and activation energy. (a) Semi-log plots of the dark currents with respect to various temperatures ranging from 260 K to 300 K . (b) Estimated activation energies versus electric fields and the corresponding dark currents at room temperature.

Figure 7 | Characterization of photo-responsivity and capacitance. The blue curve is the measured photo-responsivity as a function of bias voltage by excluding the optical insertion loss, including fiber coupling, taper and waveguide propagation losses. The red curve is the measured total capacitance as a function of bias voltage, which is slightly larger than the calculated junction capacitance of 7 fF. The input optical power is 800 μ W at 1310 nm wavelength.

forth (from forward bias to reverse bias and vice versa) and didn't show a hysteresis effect. The photo-responsivity is stable even if the device is operated for more than 1 hour. Overall, the measured device performances are comparable to or even better than those reported for the state-of-the-art Ge/Si photodiodes made by hetero-epitaxy techniques. All these properties make this device an excellent candidate for 25 Gb/s high-speed optical interconnect applications and beyond, and opens up new possibility in preparing high-quality heterojunctions between multi-materials through this self-assembled microbonding approach.

Methods

Fabrication of the Ge/Si heterojunction photodiode. A 6-inch silicon-on-insulator (SOI) substrate with 0.5- μ m device Si and 3- μ m buried oxide was cleaned and n-type doped via ion implantation of phosphor, with a concentration of $3 \times 10^{18} \text{ cm}^{-3}$. The substrate was then deposited with a SiO_2 layer of 50 nm by low pressure chemical vapor deposition (LPCVD). RMG seed windows were opened selectively by wet etching the SiO_2 until the device Si exposed for seeding Ge lateral epitaxial growth. Prior deposition of a Ge film, a 3-nm Si adhesion layer was in-situ primed. Both the Si

Figure 8 | High-frequency measurement on photodiode bandwidth at 1310 nm wavelength. A Network Analyzer (E8361C, Agilent Technologies Inc.) is used to investigate the frequency response.

and Ge layers were deposited by electron-gun evaporation in vacuum at room temperature. The Ge thickness is 0.3 μ m or 0.7 μ m, depending on different photodiode specification. The Ge beams, covering the seed windows, were defined by inductively coupled plasma (ICP) etching with Cl_2 and HBr as process gases. A thick cap oxide was coated by plasma enhanced chemical vapor deposition (PECVD) to enclose the whole Ge structure. Rapid thermal annealing (RTA) at 950°C for 4 sec was employed to melt Ge. The melted Ge re-crystallized laterally, starting from the Si seed window when the RTA system cooled down. The misfit threading dislocation defects at Ge-Si interface were necked around the step corner of the Si seed window. To bond the Ge beams on the Si waveguide, the enclosed oxide was removed by immersing the wafer in a buffered oxide etchant (BOE) solution where the Ge beams were released. As leaving out of the solution, the Ge beams were immediately adhered on the device Si layer via surface tension force. Post annealing at 400°C for 1 hr in vacuum ($< 1 \times 10^{-6}$ torr) was applied to strengthen the bonding interface. A 30-nm amorphous Si layer was deposited and covered the Ge beam for surface passivation. Next, the Si rib waveguide was defined by dry etching for light coupling. Meanwhile, the seed window was etched away to avoid leakage current directed from the Ge beam to Si substrate during operation. The waveguide rib is 3 μ m in width and 0.4 μ m in height. Finally, inter-layer dielectric was deposited and the via holes were opened. After p-type Ge doping ($> 2 \times 10^{19} \text{ cm}^{-3}$), nickel silicide (a 15 nm of Ni layer and 400°C annealing) process and metallization ($\text{TiN}/\text{AlSiCu}/\text{TiN}/\text{Ti}$) were consecutively carried out to complete the devices fabrication.

Measurement of the photodiodes. Devices were diced into chips, where the chip edges were polished for light coupling from a lensed single-mode fiber butt-coupled to the Si waveguide. The input polarization is transverse-electric (TE); in this case, the polarization is parallel to the chip surface. Agilent B1500A Semiconductor Device Parameter Analyzer is utilized to measure the I-V and C-V characteristics of the device. Operation bandwidth is characterized by measuring the S21 parameter through a network analyzer (Agilent co. E8361C). The bias electrodes are terminated to a standard GSG pad probed by a 50-Ohm RF probe (Air Coplanar Probe, CascadeMicrotech co.). We used a RF amplifier (MIREQ) after the photodiode. The optical signal is generated through a high-speed external modulator (Photline). All these components including cables and the network analyzer can be operated beyond 20 GHz. Before testing the fabricated photodiode, we calibrated the bandwidth of the whole link by replacing device under test (DUT) with a high-frequency commercial photodiode.

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Acknowledgments

The authors would like to thanks Prof. S. Hsu from National Tsing Hua University for the assistance of high-frequency measurement. The research work is funded by National Tsing Hua University (100N7080E1) in Taiwan, ROC and Intel Corporation (101A0375N6) in USA.

Author contributions

M.C.M.L. perceived the idea of microbonding through surface tension; C.K.T., W.T.C. and K.H.C. fabricated and measured the Ge/Si heterojunction photodiodes; C.K.T., H.D.L., Y.K., N.N. and M.C.M.L. designed the device; C.K.T., Y.K., N.N. and M.C.M.L. prepared the manuscript; N.N. and M.C.M.L. supervised the research project.

Additional information

Competing financial interests: The authors declare no competing financial interests.

How to cite this article: Tseng, C.-K. *et al.* A self-assembled microbonded germanium/silicon heterojunction photodiode for 25 Gb/s high-speed optical interconnects. *Sci. Rep.* **3**, 3225; DOI:10.1038/srep03225 (2013).

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