

## Gate-stack engineering of self-organized nanospherical Ge-gate/SiO<sub>2</sub>/Si<sub>1-x</sub>Ge<sub>x</sub>-channel on Si (100) and Si (110) for Ge MOS devices

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### Abstract

We report the first-of-its-kind, self-organized gate-stacking heterostructure of Ge-nanosphere (NP) /SiO<sub>2</sub> /SiGe-shell fabricated in a single step through selective oxidation of a SiGe nano-patterned pillar over buffer layers of Si<sub>3</sub>N<sub>4</sub> on Si substrates. Process-controlled tunability of the Ge-NP size (10–120 nm), the SiO<sub>2</sub> thickness (2.5–5.0 nm), and as well the SiGe-shell thickness (2–22 nm) has been demonstrated over Si (100) or (110) substrates. Detailed morphologies and structural properties of the Ge-NP/SiO<sub>2</sub>/SiGe-shell stacking structures were assessed. Single-crystalline Si<sub>1-x</sub>Ge<sub>x</sub> shells with a Ge content as high as ( $x = 0.85$ ) in a compressive stress state of 2.2% are achievable in our self-aligned gate-stack heterostructure, enabling a practically-achievable core building block for Ge-based MOS nano-electronic and photonic applications.

### 1. Introduction

Relentless miniaturization of feature sizes for CMOS devices has been widely pursued in order to boost IC performance. Aggressive downscaling into nanometer scale, however, is of formidable showstoppers not only for the process complexity and nonuniformity but also due to fundamental quantum limitation. In line with the development of exquisite process technology for continuing the downscaling track, the exploration of new materials, novel device structures, and innovative device architectures by leveraging on the wealth of CMOS technology know-how and infrastructures are highly desirable.

The inclusion of thin, strained layers of Si<sub>1-x</sub>Ge<sub>x</sub> or Ge into Si CMOS technology is one of preeminent approaches to boost the performance of both MOSFETs and MOS-photonics built on the Si platform. Recently, we have demonstrated a unique gate-stacking structure for Ge MOS devices consisting of a self-organized SiO<sub>2</sub>/Ge-NP/SiO<sub>2</sub>/SiGe-shell over the Si(100) substrate [1]. Our approach is primarily based on the exquisite control available through lithographic patterning combined with the selective oxidation of Si<sub>1-x</sub>Ge<sub>x</sub> nano-pillars over buffer layers of Si<sub>3</sub>N<sub>4</sub> deposited over the Si substrates. Remarkably our MOS gate-stack structure is generated in a single-step process, effectively eliminating complicated microfabrication processes such as surface treatments and cleaning prior to the deposition of dielectrics onto the Ge. The good crystallinity of the Ge NPs is corroborated by the clear lattice fringes and sharp diffraction spots from HRTEM and selected-area diffraction (SAD) observations. Importantly, our MOS gate stack possesses good tunability for the Ge-NP size, the interfacial SiO<sub>2</sub> thickness, and the SiGe-shell thickness, thus

providing a core building block for practical Ge-based MOS devices. Thereby, we have further advanced this unique heterostructure for the production of Al/SiO<sub>2</sub>/Ge-NP/SiO<sub>2</sub>/SiGe nanocrystal transistors with good charge retention and endurance [1] as well as for the fabrication of ITO/SiO<sub>2</sub>/Ge-NP/SiO<sub>2</sub>/SiGe phototransistors with superior photoresponsivity and very low dark current [2].

In this paper, we further advanced the controllability over the chemical composition and strain states of the SiGe-shells over SOI (100) and (110) substrates in order to further exploit high-performance Ge MOS nanoelectronics and nanophotonics.

### 2. Experimental results and discussion

Process flow and the corresponding transmission electron microscopy (TEM)/energy-dispersive x-ray spectroscopy (EDX) micrographs of Ge-NP/SiO<sub>2</sub>/SiGe-shell over Si substrates are summarized in Fig. 1. Both thicknesses of the interfacial SiO<sub>2</sub> layer and the Si<sub>1-x</sub>Ge<sub>x</sub> shell appear to increase with the Ge NPs penetrating deeper into the Si substrates when increasing oxidation time, and such a dependence is greatly enhanced when the crystal orientation of the Si substrates is changed from (100) to (110) (Fig. 2). As elaborated in our previous reports [4], the formation of the interfacial SiO<sub>2</sub> layer is an exquisitely-controlled dynamic equilibrium that exists between the concentration of Si interstitials emitted from Si substrates and external oxygen flux. The higher oxidation rate on the Si (110) crystal plane is because there are a higher number of surface atoms/chemical bonds than the (100) plane (available bonds:  $9.59 \times 10^{14} \text{ cm}^{-2}$  for Si(110) versus  $6.77 \times 10^{14} \text{ cm}^{-2}$  for Si(100)).

The formation of a thin, cup-shaped Si<sub>1-x</sub>Ge<sub>x</sub> shell that is conformal with the Ge NP and the Si substrate is attributable to the Ge atoms migrating from the Ge NP and dissolving within the Si substrate. Figure 3(a) shows the Raman spectra for the variable-sized Si<sub>1-x</sub>Ge<sub>x</sub> shells over Si(110). Considerable redshifts for both the longitudinal optical (LO) Ge-Ge phonon lines ( $295 - 300 \text{ cm}^{-1}$ ) and the Si-Si lines ( $505 - 510 \text{ cm}^{-1}$ ) were measured on the 50 - 120nm-long SiGe shells compared to the Raman lines of  $301.5 \text{ cm}^{-1}$  for bulk Ge and  $520 \text{ cm}^{-1}$  for bulk Si, respectively. We are able to extract the Ge content and strain states for each Si<sub>1-x</sub>Ge<sub>x</sub> shell from the corresponding Raman shifts. A higher Si interstitial flux released from (110) Si crystal plane in combination with a lower diffusion coefficient for Ge within (110) Si crystal planes lead to the resulting Si<sub>1-x</sub>Ge<sub>x</sub> shells over (110) Si surface having a lower Ge content of  $x = 0.3 - 0.35$  in comparison to the Si<sub>1-x</sub>Ge<sub>x</sub> shell with higher Ge content of  $x = 0.6 - 0.85$  over Si(100) (Figure 3(b)). A lattice-constant mismatch between Ge and Si also leads to a compressive strain of -1.5% and -2.5% for

the  $\text{Si}_{0.7}\text{Ge}_{0.3}$  shells over (110) Si and the  $\text{Si}_{0.15}\text{Ge}_{0.85}$  shells over (100) Si, respectively. The large compressive strain states for the SiGe shells over Si(100) and over Si(110) are further experimentally evidenced by the top-view SAD examinations as shown in Figure 4.

### 3. Conclusion

We report the fabrication of self-organized gate-stacking heterostructure of Ge-nanosphere (NP)/ $\text{SiO}_2$ /SiGe-shell over Si(100) and Si(110) substrates. Good tunability of the geometrical conditions for the Ge-NP size (10–120 nm), the  $\text{SiO}_2$  thickness (2.5–5.0 nm), and the SiGe-shell thickness (2–22 nm) has been demonstrated over Si (100) or (110) substrates. Ge contents of  $x$

$= 0.6–0.85$  with a compressive strain of  $-2.5\%$  and  $x = 0.3–0.35$  with a strain of  $-1.5\%$  for the resulting  $\text{Si}_{1-x}\text{Ge}_x$  shells over the Si(100) and over the Si(110), respectively, were extracted from the red shifts in Ge-Ge and Si-Si phonon lines. This indicates that our self-aligned gate-stack heterostructure, enabling a practically-achievable core building block for Ge-based MOS nano-electronic and photonic applications.

### 4. References

- [1] W. T. Lai et al., *Nanoscale Res. Lett.*, 10, 224, 2015.
- [2] M. H. Kuo et al., *Optics Lett.*, 40, 2401, 2015.

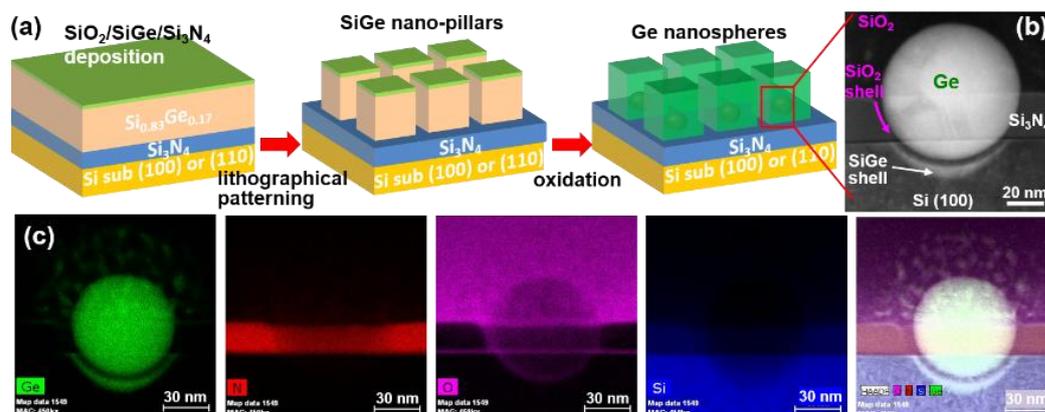


Fig. 1 Heterostructure of Ge NP/ $\text{SiO}_2$ /SiGe shell produced by thermally oxidizing SiGe nanopillar over buffer layers of  $\text{Si}_3\text{N}_4$  on Si(100) substrate at  $900^\circ\text{C}$  for 25 min. followed by annealing at  $875^\circ\text{C}$ , 5min in an  $\text{H}_2\text{O}$  ambient. (a) schematics of experimental fabrication procedure, (b) STEM and (c) EDX mapping micrographs.

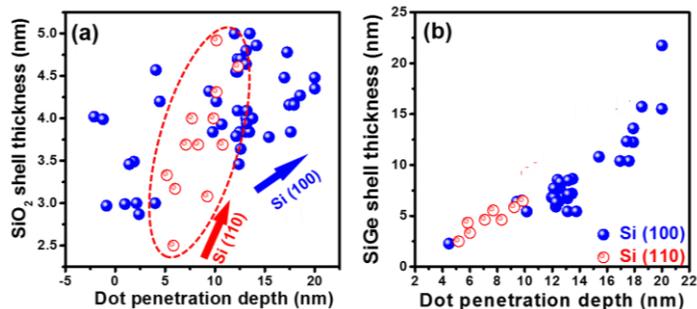


Figure 2 Thicknesses of (a)  $\text{SiO}_2$  shell and (b) SiGe shell for the heterostructure of Ge dot/ $\text{SiO}_2$ /SiGe shell formed following  $900^\circ\text{C}$  in an  $\text{H}_2\text{O}$  ambient.

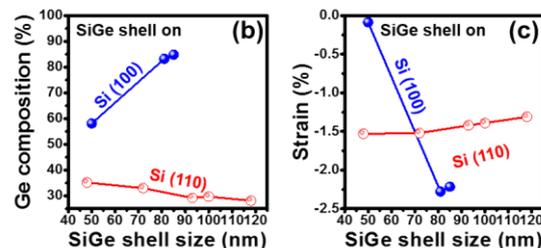
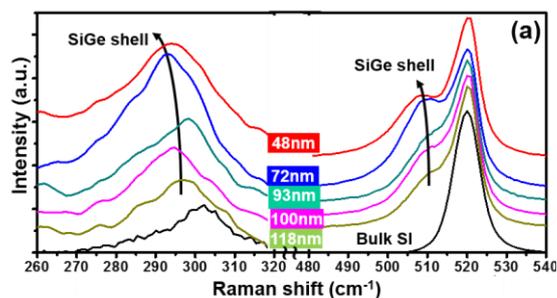


Figure 3 (a) Raman spectra for SiGe shell on SOI (110), (b) extracted Ge composition and (c) compressive strain for the SiGe shells over SOI (100) and SOI (110) substrates.

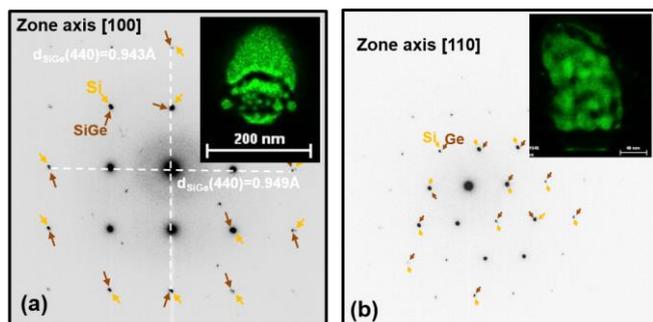


Figure 4 Top-view SAD for the SiGe shells over (a) SOI (100) and (b) SOI (110) substrates.