Dewetting-Induced Formation and Optical Properties of Arrays of Low-Ge-Content SiGe Mie-Resonators on Si (100) Surface

Vladimir Poborchii¹, Alexander Shklyaev², Leonid Bolotov¹, Noriyuki Uchida¹ and Tetsuya Tada¹

¹ Nanoelectronics Research Institute, National Institute of Advanced Industrial Science and Technology, 1-1-1 Higashi, AIST Central-5, Tsukuba 305-8565, Japan

Phone: +81-298-491633, e-mail: vladimir.p@aist.go.jp

²A.V. Rzhanov Institute of Semiconductor Physics, SB RAS, Novosibirsk 630090, Russia

Abstract

Submicron-sized high-index Mie-resonators attract significant interest due to their capabilities to manipulate, redirect and concentrate the light. 2D metamaterials consisting of arrays of such resonators on device surface can be used in the integrated optics, photodetectors, solar cells and other applications. Here, we report optical properties of nearly regular Mie resonator arrays prepared on Si surface using a simple and low-cost method. We deposited Ge on Si (100) surface at elevated temperature ~ 900 C. Owing to dewetting, we obtained high-density 2D arrays of submicron lens-like SiGe islands with low Ge content. The islands display Mie resonances, antireflection and light concentration effects in the visible - near infrared range. Such SiGe island arrays are promising metasurfaces for photodetectors and solar cells.

1. Introduction

High-refractive-index (n) submicron-sized dielectric particles attract much attention due to their ability for Mie-resonance scattering, redirection, concentration and manipulation of electromagnetic radiation with the wavelength (λ) of the order of the particle size $d \sim \lambda/n$. Silicon with $n \sim 3.5 - 5$ in the infrared (IR) - visible spectral range is a suitable materials for such Mie-resonance engineering. Si particle arrays can work as nano-antennas, non-linear optical elements and flat photonic devices. One can use them to enhance performance of photodetectors, optical sources, thermal emitters, solar cells etc. [1]. In this work, low-Ge-content SiGe visible-near-IR Mie-resonator island arrays are formed at high temperature on the Si (100) surface due to dewetting. High density and lens-like shape of the islands provide broadband antireflection and light concentration needed for photodetectors and solar cells.

2. Experimental and Theoretical Methods

A bar-like Si substrate (Fig. 1a) was heated by the electric current up to ~ 900° C in the central part while areas close to the bar ends with electric contacts displayed slightly lower temperature. During Ge deposition, nearly regular 2D arrays of submicron Si_{1-x}Ge_x islands were obtained similar to [2]. The regularity was high for x < 0.15 but it weakened for x > 0.15. The island arrays were characterized using scanning electron microscopy (SEM), atomic force microscopy. Raman microscopy and micro-optical reflec-

tion/scattering spectroscopy. Optical properties of Si particles with the shapes of disk and segment of sphere were calculated using discrete dipole approximation with ADDA code [3].





3. Results

Islands with the lens-like shape (Fig. 2a) and low Ge content $x \sim 0.1$ are shown in Fig. 2.



Fig. 2 (a) SEM image of the convex-lens-shape SiGe islands.with the diameter $D \sim 500$ nm and height $H \sim 115$ nm. (b) Raman shift and Ge content vs. position across SiGe island.

Raman measurements (Fig. 1b and 2b) were made with the excitation $\lambda = 364$ nm, corresponding to the penetration depth ~ 10 nm, and 100x N.A.0.95 lens, providing spatial resolution ~ 250 nm. Rather sharp Si_{1-x}Ge_x Raman band (Fig. 1b) showed strong dependence on *x* and light polarization proving good monocrystalline quality of the islands and their [110] axis orientation parallel to that of the Si substrate. Reduction of Ge content from the island center to its sharp edge was detected (Fig. 2b).

Fig. 3a shows antireflection effect produced by the SiGe island arrays. Normal-incidence reflection is reduced by 7-10 times in the area 1 compared to Si and 4-5 times in the areas 3 and 2. Fig. 3b shows Raman spectra taken from the corresponding areas with $\lambda = 561$ nm and few-micron probe size. The Si substrate band at 520-521 cm⁻¹ dominates over

the SiGe island band due to the large penetration depth $\sim 1 \ \mu m$ of the 561 nm light and it is enhanced in the SiGe island areas compared to that of bare substrate.



Fig. 3. Reflection compared to Si substrate (a) and Raman (b) spectra of the SiGe island areas 1, 2 and 3 indicated in Fig. 1. Raman measurement was done with $\lambda = 561$ nm and 4x lens with N.A. 0.16 focusing light into a few micron area.



Fig. 4. (a) Raman intensity/shift maps of ~ $5\mu m \times 5\mu m$ area taken with $\lambda = 561$ nm and 100x lens with N.A. 0.95 providing spatial resolution ~ 350nm; (b) ADDA simulation of the normal-incident 560 nm light propagation through Si sphere segment (D = 500 nm and H = 115 nm) located on the top of ~ 3.4 µm thick Si box. Light is polarized along the *Y* axis (*E*//*Y*).

Fig. 4a shows Raman intensity/shift maps between areas 2 and 3 of Fig.1 taken with $\lambda = 561$ nm and high N.A. lens. Clearly, Si substrate signal is enhanced under SiGe islands up to a factor of ~ 3 at the island with coordinates: ~63µm, ~55µm. Island-induced light-concentration effect is demonstrated in Fig. 4b using ADDA simulation, optical constants of the island and Si substrate being the same. SiGe-island-induced tensile stress of Si substrate is displayed in the substrate band downshift compared to unstressed Si (520.5 cm⁻¹). Substrate compressive stress causing Si band upshift up to ~ 520.7 cm⁻¹ is observed in the areas between the islands.

Laser power (P) dependencies of the substrate Raman shift under SiGe island and with no island are shown in Fig. 5a. Nearly 2-fold SiGe-island-induced increase in the heating-induced downshift slope is a clear indication of the light concentration. Extrapolation of the Raman shift values to P = 0 reveals stress-induced Si band downshift ~0.34 cm⁻¹ that corresponds to biaxial tensile stress ~ 70 MPa.

A variety of island colours is displayed in the white-light back scattering image of SiGe islands obtained with a long-working-distance 50x lens with N.A. 0.5 (Fig.5b). The colours are associated with Mie resonances observed in the experimental and theoretical scattering spectra (Fig. 6). Both spectra display Mie resonances showing higher activity for $E \perp Y$ polarization. Our calculations show that the band at ~ 740 nm corresponds to off-plane electric dipole resonance while higher frequency peak corresponds to a combination of multipole resonances. In-plane electric dipole and off-plane magnetic dipole resonances, active without substrate in the range 1000-1200 nm, are broadened due to strong coupling with the substrate and seen as background.



Fig. 5. (a) 561 nm laser power dependencies of the Si substrate band Raman shift with no SiGe islands (squares) and under SiiGe island (triangles); (b) back-scattering image of SiGe islands with the light incident at ~ 60° angle to the normal (*Z* axis) of Si surface for *E*//*Y* and *E* \perp *Y* polarizations.



Fig. 6. Experimental (a) and theoretical (b) light scattering spectra of a single island for E//Y and $E \perp Y$ light polarizations.at the incident angle of 60 °. Theoretical calculation was done for Si sphere segment with D = 500nm and H = 115nm

Conclusions

High-density low-Ge-content monocrystalline SiGe visible-near-IR Mie-resonator lens-like island arrays were fabricated on Si (100) surface using dewetting. Our optical study shows that the islands produce pronounced antireflection and light concentration effects. The arrays are promising photodetector and solar-cell metasurfaces.

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