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The influence of growth modes on the characteristics of germanium-silicon microresonators on a thick silicon oxide layer

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In this study dependences of the structural parameters of germanium microresonators formed on an oxidized silicon surface (average island size, island size distribution, island height-to-diameter ratio, and island surface density) on post-growth annealing conditions were determined. Optical characteristics of the resulting heterostructures with microresonators were investigated. Their potential for use as absorbing structures as well as antireflection coatings for certain wavelengths was demonstrated. Methods for controlling the geometric and optical characteristics of microresonator ensembles by varying the parameters of their epitaxial synthesis were proposed.

Keywords: microresonators, silicon, germanium, molecular beam epitaxy, atomic force microscopy, transmission spectra, reflectance spectra.

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Introduction

Microresonators (Mie resonators) are capable of localizing and enhancing the electromagnetic field at certain resonant wavelengths. When integrated with quantum dots, such structures provide a substantial enhancement of the optical response, which increases the efficiency of detecting weak signals in photosensitive devices [1, 2].

An important factor determining the functional capabilities of microresonators is their antireflective properties, which make it possible to increase the efficiency and sensitivity of optoelectronic devices when integrated into active structures. The placement of microresonators on a surface leads to a significant reduction in the reflection coefficient in certain spectral ranges, which are set by their geometric parameters. This effect is due to the occurrence of Mie scattering

during the interaction of electromagnetic radiation with surface inhomogeneities whose characteristic dimensions are comparable to the wavelength of the incident radiation [3].

As a result of Mie scattering, the character of radiation reflection from the surface changes: instead of predominantly specular reflection, diffuse scattering arises, in which part of the incident radiation is redistributed in various directions. At the same time, a significant fraction of the energy propagates along the surface of the structure, promoting more efficient input of radiation into the material. Such a mechanism leads to an increase in transmission and a reduction in reflection losses over a broad spectral range [1].

Molecular beam epitaxy (MBE) makes it possible to obtain pure nanostructures with a minimal number of defects [4]. Reflection high-energy electron diffraction (RHEED) is used to

analyze the surface morphology of the samples [5]. RHEED makes it possible to monitor the surface morphology during growth with an accuracy of high precision (less than one monolayer (ML)) [6]. Control of epitaxial processes by changing the temperature and deposition rate and by using special substrates makes it possible to create self-organized structures with the required parameters and desired properties [7]. Recently, particular attention has been paid to the development and epitaxial creation of photosensitive elements [8, 9] based on germanium-silicon microresonators, including the creation of antireflective coatings on their basis [10, 11].

Methods

In the present work, germanium microresonators were created on an oxidized silicon surface by molecular beam epitaxy followed by annealing under ultrahigh vacuum conditions. Si(001) wafers were used as substrates for germanium deposition. The experimental studies were carried out on a Katun-100 MBE setup. After the pre-epitaxial preparation of the Si(001) wafer, a thick oxide layer of SiO₂ (about 100 nm) was deposited on it by the magnetron method. Then, a GeSi solid solution of various thicknesses with a Ge percentage content of 30% was deposited on the oxidized substrate. The deposition rate was determined by the method of reflection high-energy electron diffraction from the intensity oscillations during the deposition of materials onto a Si(001) substrate without an oxide layer. Deposition occurred at a temperature of 400 °C to exclude Ge segregation and create a uniform layer. After the deposition of the germanium and silicon layers, the obtained structures were annealed at a temperature of 800 °C with various annealing durations.

The state of the surface during growth was monitored using the method of reflection high-energy electron diffraction. After synthesis, the surface morphology was studied by atomic force microscopy. The optical characteristics of the obtained structures were studied by the method of optical spectrometry for diffuse reflection using a Shimadzu UV-3600 Plus spectrophotometer. The measured spectra were compared with the

calculated ones obtained in the Lumerical environment by the finite-difference time-domain method.

Results

Judging by the data of the RHEED studies carried out during the entire experiment, the GeSi film before annealing had an amorphous structure, as evidenced by the presence of two broad blurred diffuse halos. During annealing, the structure became polycrystalline: Debye–Scherrer rings were formed on the RHEED patterns. Upon completion of annealing, reflections additionally appeared on the patterns, corresponding to transmission diffraction from the periodic structure.

As a result of the annealing of structures with a deposited layer of silicon-germanium solid solution on an oxidized silicon surface, an ensemble of nanoislands was formed with characteristic sizes of 150–250 nm and a height of 100–250 nm. Figure 1 shows an SEM image of a sample with a deposited solid solution layer (effective thickness 33 nm) that was annealed at a temperature of 800 °C for 1 hour. Analysis of the image makes it possible to estimate the surface density ($\sim 1 \times 10^9 \text{ cm}^{-2}$) and the size distribution of the islands. The average size of the islands under these annealing conditions was 200 nm.

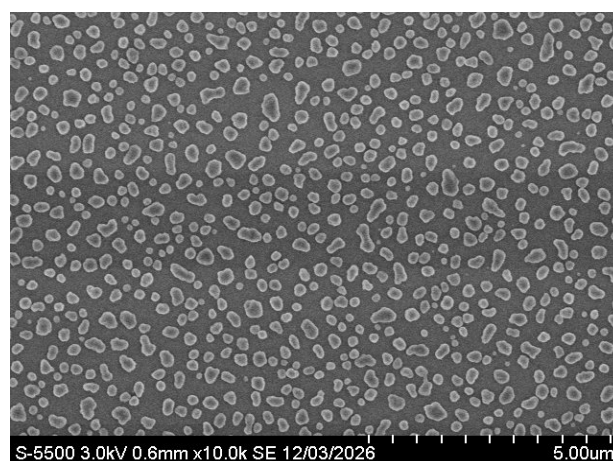


Fig. 1. SEM image of a sample with germanium-silicon microresonators (effective thickness 33 nm) on magnetron silicon oxide

For a more detailed study of the geometric characteristics of the obtained nanoislands

(including their height), the samples were examined by atomic force microscopy in the semi-contact mode using a cantilever with a tip radius of 2 nm. The study of the morphological characteristics of the formed microresonators by atomic force microscopy made it possible to determine the distributions of height and base diameter, as well as to estimate their surface density. Figure 2 shows the dependences of the average base diameter (d) and the height-to-diameter ratio (h/d) on the thickness of the deposited silicon-germanium layer for samples annealed at 800 °C for 1 hour.

In accordance with Figure 2, with an increasing effective thickness of the deposited solid solution, the island size increases. The island diameter d increases almost linearly, while

the height-to-diameter ratio, h/d , grows nonlinearly, gradually approaching unity.

Experiments on varying the parameters of post-growth annealing showed that an increase in the annealing temperature or duration leads to an increase in the diameter and a decrease in the parameter h/d .

To study the optical response of the structures, transmission and diffuse reflection spectra were recorded over a broad spectral range. As an illustration, Figure 3 presents the diffuse reflection spectra of two samples with average island sizes of 150 and 200 nm. A clear resonant character in the reflection spectra of such nanoislands is observed, as well as a substantial dependence of the spectral profile on the sizes of the microresonators.

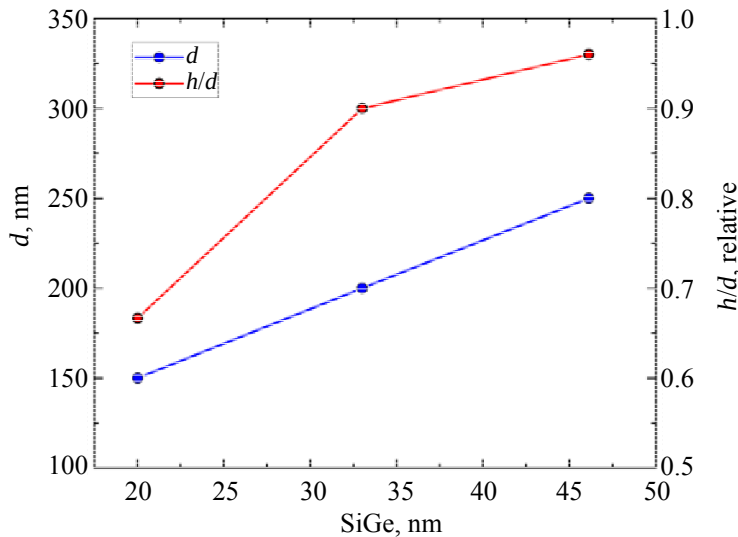


Fig. 2. Dependence of the base diameter d (blue curve) and the height-to-base-diameter ratio h/d (red curve) on the thickness of the deposited silicon-germanium solid solution

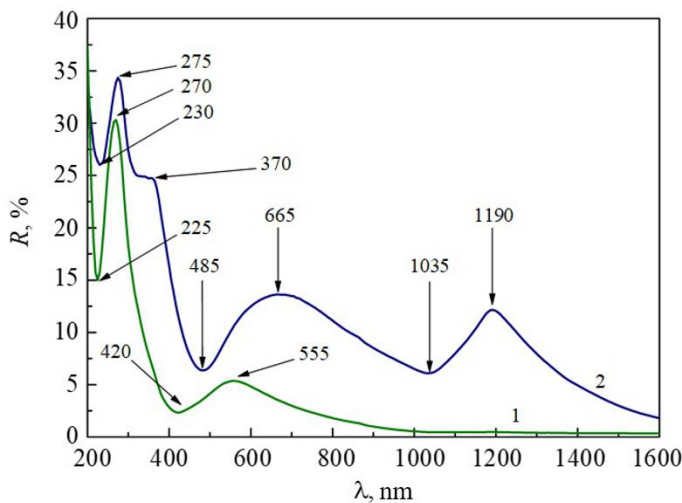


Fig. 3. Experimental diffuse reflection spectra of structures with silicon-germanium microresonators on a thick silicon oxide layer with an average size of 150 nm (curve 1) and 200 nm (curve 2)

In the reflection spectra, alternating maxima and minima are observed, caused by the

excitation of Mie resonances in the nanoislands. At the same time, for the initial silicon surface,

the contribution of diffuse reflection is negligible, since the reflection is predominantly specular in nature. Outside the resonance regions, the transmission spectra of the structures with microresonators practically coincide with the transmission of the initial silicon substrate.

The results of numerical modeling of the optical characteristics of layers with microresonators having diameters of 150 and 200 nm and a height-to-diameter ratio $h/d = 1$ are

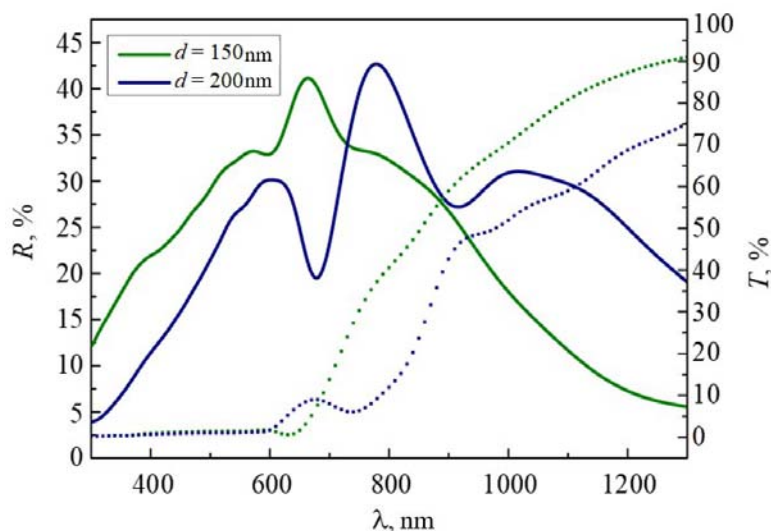


Fig. 4. Calculated reflection spectra (solid lines) and transmission spectra (dashed lines) of a layer with microresonators having diameters of 150 and 200 nm

Comparison of the experimental and calculated data (Figures 3 and 4) demonstrates qualitative agreement in the presence of intensity extrema only in a narrow wavelength range of 550–650 nm. The observed differences in the absolute values of the reflection and transmission coefficients, as well as in the number and width of the resonance peaks, are due to the inevitable spread in the sizes of the formed islands, which leads to smoothing of the spectral features.

Measurements of the reflection spectra performed at various angles of incidence and radiation detection did not reveal a significant angular dependence of the intensity. This indicates the predominantly diffuse character of reflection in structures with GeSi microresonators on an oxidized silicon surface. Analysis of samples with different values of h/d shows that a reduction in reflection and an increase in transmission are achieved with an increase in the ratio of the height of the microresonators to the diameter of their base. This is due to the improvement of the conditions for the simultaneous manifestation of electric and magnetic resonances in such structures [11].

presented in Figure 4. In the calculated spectra, the features associated with size resonances manifest themselves more clearly. It is shown that an increase in the island diameter leads to the appearance of additional resonant extrema in the reflection spectra. Nevertheless, the calculated data so far provide only preliminary information about the real spectra, since they do not take into account the large spread in islands size that inevitably exists in the grown samples.

Conclusion

As a result of the study, the dependences of the structural parameters of the formed germanium microresonators on a thick silicon oxide layer (average island size, island size distribution, height-to-island-diameter ratio, surface density of islands) on the post-growth annealing regimes were determined. The optical characteristics of the obtained heterostructures with microresonators were also determined. The prospects of their application not only as absorbing structures, but also as antireflective coatings for certain wavelengths are demonstrated. Ways to control the geometric and optical characteristics of the ensemble of microresonators by changing the parameters of their epitaxial synthesis are proposed.

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