St. Petersburg Polytechnic University Journal. Physics and Mathematics. 2024. Vol. 17. No. 3.1
Научно-технические ведомости СПбГПУ. Физико-математические науки. 17 (3.1) 2024

Conference materials
UDC 535
DOI: https://doi.org/10.18721/JPM.173.121

Resonant scattering of silicon nanopillars for nonlinear optics

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Abstract. This article summarizes the findings of a study on resonant scattering from single silicon nanopillars on a native substrate in the visible and near infrared spectral ranges. The study utilizes numerical simulation finite-difference time-domain method to investigate the effects of lateral and vertical dimensions of the pillars on their scattering behavior. The results show that manipulating the dimensions can shift resonance modes and enhance scattering intensity. Various pillars design variations are explored, including different lengths and radii, with the aim of optimizing scattering intensity for up-conversion devices.

Keywords: resonant scattering, silicon pillars, nonlinear optics

Funding: Ministry of Science and Higher Education of the Russian Federation (Grant FSRM-2023-0009).

Citation: Kondratev V.M., Kuznetsov A., Zavyalova E.S., Anikina M.A., Bolshakov A.D., Resonant scattering of silicon nanopillars for nonlinear optics, St. Petersburg State Polytechnical University Journal. Physics and Mathematics. 17 (3.1) (2024) 110–114. DOI: https://doi.org/10.18721/JPM.173.121

Материалы конференции
УДК 535
DOI: https://doi.org/10.18721/JPM.173.121

Резонансное рассеяние одиночных кремниевых наностолбиков для нелинейной оптики

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Аннотация. Данная работа посвящена исследованию резонансного рассеяния одиночных кремниевых наностолбиков для решения задач нелинейной оптики. Показаны оптимальные геометрии кремниевых столбиков, обладающие максимальной интенсивностью рассеяния, которые могут быть использованы для создания устройств нанофотоники.

Ключевые слова: резонансное рассеяние, кремниевый столбик, нелинейная оптика

Финансирование: Министерство науки и высшего образования Российской Федерации (грант № FSRM-2023-0009).

Ссылка при цитировании: Кондратьев В.М., Кузнецов А., Завьялова Е.С., Аникина М.А., Большаков А.Д. Резонансное рассеяние одиночных кремниевых наностолбиков для нелинейной оптики // Научно-технические ведомости СПбГПУ. Физико-математические науки. 2024. Т. 17. № 3.1. С. 110–114. DOI: https://doi.org/10.18721/JPM.173.121

Introduction

Silicon micro- and nanostructures, such as pillars and wires [1, 2], are commonly employed in photonics and sensor applications [3–8]. Resonant scattering from silicon pillars on a substrate in the visible and near infrared spectral ranges is of particular interest for developing nonlinear optical devices. This study focuses on investigation of the resonant scattering of individual silicon columns to address challenges in the field of nonlinear optics. We use numerical modeling to study the interaction between light and silicon nanopillars with the goal of optimizing the structures' geometry to enhance the second harmonic (SH) response. By carefully analyzing the impact of various parameters on the nanopillar structures, we were able to determine the optimal geometry. Our results demonstrate the importance of precise control over the geometry of the nanopillars in order to achieve enhanced SH generation. These findings have important implications for the development of efficient photonic devices and applications.

Materials and Methods

To optimize the second harmonic generation (SHG) in Si pillars the numerical simulation was utilized. The calculations were carried out with an aid of finite-difference time-domain method (FDTD) according to Yee algorithm in Ansys Lumerical software. Single pillars were modeled as cylinders of different height and radius on native Si substrate. The spatial mesh step was 5 nm and the boundary conditions were absorptive (perfectly-matched layer, PML) to avoid artificial reflection in the simulation region. The excitation was simulated by the broadband plane wave source located at a 1-micron distance from the pillar edge directed perpendicularly to the substrate. To achieve more precise evaluation of the scattered field it was monitored only above the structure to be in agreement with the dark-field spectroscopy experimental setup collecting backscattered signal. The calculations were provided in 500–1300 nm spectral range. Geometry of the problem is demonstrated in Fig. 1.

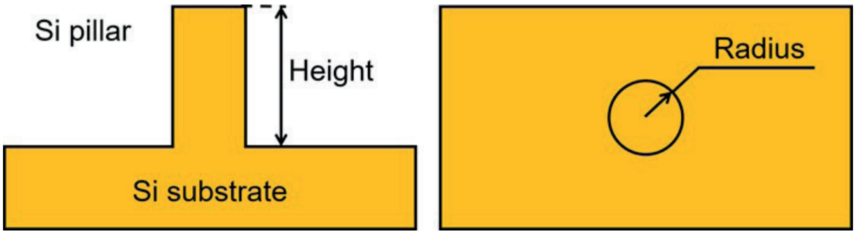

Fig. 1. Schematic of the single Si pillar for simulation

Results and Discussion

In this work we investigated the possibility of the SHG from single Si pillars. Si lattice is known to posses the inversion symmetry and second-order dielectric permeability equals zero. But, on the other hand, in the vicinity of the surface the symmetry is no longer preserved so, that is why we can achieve second-order nonlinear response. Also, according to the experimental works [4–7] such types of structures are synthesized by etching which affects the surface layers which undergo amorphization breaking the inversion symmetry. The first step to analyze the possibility of the SHG in single nanostructures and metasurfaces is to calculate its scattering spectra and its dependencies from the geometry. The main goal is to match scattering peaks with pump and SHG spectral position [8]. For the structure under consideration, we estimate the SHG signal at 550 nm. To find resonant modes we calculated scattering spectra in 500–1300 nm spectral range for pillars height of 0.35, 0.4, 0.45, 0.5, 1.2, 1.4, 1.6, 1.8 and 2 μm in the range of radii 50–600 nm. In Fig. 2 the scattering spectra intensity maps for different diameters and heights of 0.45 and 1.8 μm are demonstrated.

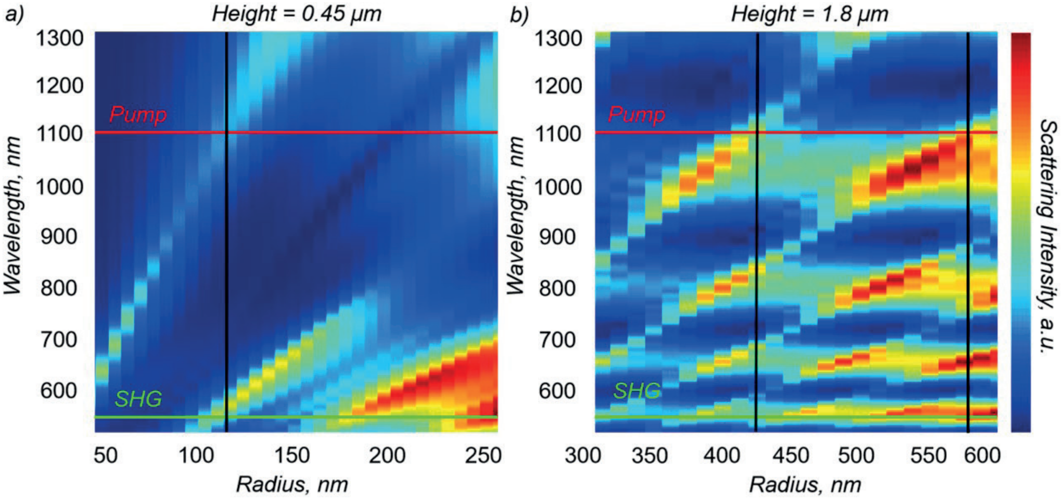

Fig. 2. Scattering spectra of the single Si pillars of different radii (*a*) 0.45 μm and (*b*) 1.8 μm tall

In Fig. 2 we can see scattering modes evolution with increase of the pillars radius. Two degrees of freedom (radius and height) allow us to precisely control the number of resonant modes and its spectral position. For example, using the pillar with the radius of 112.5 nm and the height of 0.45 μm provides the perfect match of two scattered modes with pump and SHG spectral lines. Instead of utilizing very small pillars which fabrication could be challenging it is evident from (Fig. 2, *b*) that we can achieve prominent resonant response from pillars higher than 1 μm and thicker than 300 nm (radius). In this case we achieve one order higher scattering intensity but the number of modes drastically increases with the increase of pillars height (Fig. 3). Additional longitudinal modes can affect the energy redistribution between them and decrease the SHG response intensity.

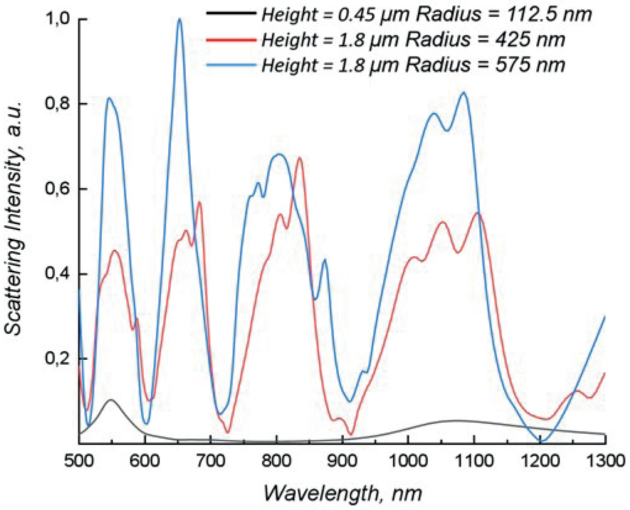

Fig. 3. Scattering spectra of the single Si pillars 0.45, 1.80 μm high and with the radii of 112.5, 425.0 and 575.0 nm

Conclusion

To sum up we demonstrate resonant scattering from the single Si pillars on the native substrate in the visible and near IR spectral ranges using numerical simulation finite-difference time-domain method. Precise control of the pillars lateral and longitudinal dimensions drastically affect the scattering behaviour of the pillar by shifting the resonant modes and changing their number. We demonstrate that there are several pillar designs having resonant features in the range of pump (1100 nm) and SHG (550 nm) lines with heights of 0.45 and 1.8 μm and radii of 112.5, 425 and 575 nm. More precise optimization should be carried out to achieve the structure with maximum scattering intensity in the spectral range of interest and it will open up the new pathways in design of the CMOS-compatible resonant up-conversion devices.

Acknowledgments

Authors thanks the Ministry of Science and Higher Education of the Russian Federation (Grant FSRM-2023-0009) for their support of the studies on the nonlinear response of silicon pillars and the identification of the underlying nature of this response.

REFERENCES

1. **Bolshakov A.D., Mozharov A.M., Sapunov G.A., Fedorov V.V., Dvoretckaia L.N., Mukhin I.S.,** Theoretical modeling of the self-catalyzed nanowire growth: nucleation-and adsorption-limited regimes. Materials Research Express. 4 (12) (2017) 125027.

2. **Dubrovskii V.G., Bolshakov A.D., Williams B.L., Durose K.,** Growth modeling of CdTe nanowires. Nanotechnology. 23(48) (2012) 485607.

3. **Bolshakov A.D., Shishkin I., Machnev A., Petrov M., Kirilenko D.A., Fedorov V.V., Ginzburg P.,** Single GaP nanowire nonlinear characterization with the aid of an optical trap. Nanoscale. 14 (3) (2022) 993–1000.

4. **Hsu C.M., Connor S.T., Tang M.X., Cui Y.,** Wafer-scale silicon nanopillars and nanocones by Langmuir-Blodgett assembly and etching, Appl Phys Lett 93 (2008).

5. **Chen W., Ahmed H.,** Fabrication of high aspect ratio silicon pillars of <10 nm diameter, Appl Phys Lett 63 (1993).

6. **Kondratev V.M., Morozov I.A., Vyacheslavova E.A., Kirilenko D.A., Kuznetsov A., Kadinskaya S.A., Nalimova S.S., Moshnikov V.A., Gudovskikh A.S., Bolshakov A.D.,** Silicon Nanowire-Based Room-Temperature Multi-environment Ammonia Detection, ACS Appl Nano Mater 5 (2022) 9940–9949.

7. **Kondratev V.M., Vyacheslavova E.A., Shugabaev T., Kirilenko D.A., Kuznetsov A., Kadinskaya S.A., Shomakhov Z.V., Baranov A.I., Nalimova S.S., Moshnikov V.A., Gudovskikh A.S., Bolshakov A.D.,** Si Nanowire-Based Schottky Sensors for Selective Sensing of NH3 and HCl via Impedance Spectroscopy, ACS Appl Nano Mater 6 (2023) 11513–11523.

8. **Makarov S.V., Petrov M.I., Zywietz U., Milichko V., Zuev D., Lopanitsyna N., Kuksin A., Mukhin I., Zograf G., Ubyivovk E., Smirnova D.A., Starikov S., Chichkov B.N., Kivshar Y.S.,** Efficient Second-Harmonic Generation in Nanocrystalline Silicon Nanoparticles, Nano Lett 17 (2017).

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Received 12.07.2024. Approved after reviewing 02.08.2024. Accepted 02.08.2024.