Optics Communications 399 (2017) 127–134

Contents lists available at ScienceDirect

Optics Communications

journal homepage: www.elsevier.com/locate/optcom

Effective optical properties of supported silicon nanopillars at telecommunication wavelengths

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ARTICLE INFO

Keywords:
Silicon photonics
Effective medium theory
Transformation optics
Optical metamaterials
High index dielectrics
Light scattering

ABSTRACT

We measure and calculate the optical response of a structure consisting of a square array of subwavelength silicon posts on a silicon substrate at telecommunication wavelengths. By the use of the reduced Rayleigh equations and the Fourier modal method (rigorous coupled wave analysis) we calculate the reflectivity of this structure illuminated from vacuum by normally incident light. The calculated reflectivities together with experimentally determined ones, are used to test the accuracy of effective medium theories of the optical properties of structured silicon surfaces, and to estimate the effective refractive index of such surfaces produced by a homogeneous layer model.

1. Introduction

It has been established that Maxwell's equations are form-invariant under geometrical transformations [1], and that the consequences of a given transformation can be interpreted in terms of modifications of the material properties involved. Thus, regions with homogeneous properties are transformed into regions whose permittivity and permeability are determined by the mathematical nature of the transformation. This property has given rise to the field of transformation optics [1], which is an emerging area of optics in which coordinate transformations are used to design structures with novel optical properties. Using such techniques, designs for cloaking [2–4], and other interesting devices [5–7] have been proposed.

The practical realization of such structures and devices is, however, quite challenging, as the media in transformed space are in general anisotropic and their electromagnetic properties are functions of position. Not surprisingly, transformation optics is usually associated with the field of optical metamaterials, which are artificial materials whose permittivity and permeability can attain values that are different from those of materials found in nature. The concept of a metamaterial is intimately related to the notion of an effective medium; it relies on the idea that when the inclusions or heterogeneities are much smaller than the wavelength, the wave propagates as in a homogeneous medium with some effective optical properties that depend on the geometry and the filling fraction of the inclusions.

Silicon and Silicon on Insulator (SOI) wafers constitute interesting platforms for experimental tests of transformation optics concepts, and for the implementation of novel designs for silicon photonics. On the one hand, silicon is a well studied material that is transparent in the near infrared and can be structured using electron beam lithography and ion etching techniques. Silicon photonics has become increasingly popular due to its natural integration with fiber optics communication links, and SOI wafers are designed to facilitate the implementation of two-dimensional integrated circuits. Additionally, the 2D nature of the photonic circuits makes the use of conformal mapping techniques [2] appropriate in their design. Conformal mappings constitute a class of two-dimensional transformations that have proved useful in the past for solving diffraction problems [8,9]. Implementing transformation optics concepts in silicon photonics is interesting from both, the conceptual and application points of view [10].

To our knowledge, however, the accuracy of the effective refractive index theories has not been tested for the kinds of structures and refractive index contrasts encountered in silicon photonics. In this paper, we explore this question for the case of silicon nanopillars over a silicon substrate. We test what are perhaps the simplest effective medium theories by comparing the measured reflectivity of fabricated samples with the results of calculations based on the Maxwell Garnett [11] and Bruggeman's [12] approaches, and through electromagnetic

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http://dx.doi.org/10.1016/j.optcom.2017.04.027
Received 16 January 2017; Received in revised form 10 April 2017; Accepted 11 April 2017
Available online 10 May 2017
0030-4018/

scattering calculations. We present calculations based on a numerical Rayleigh method that, although it has some limitation on the height of the pillars that can be dealt with, has the advantage of being computationally fast. The other method employed for the calculations is the rigorous coupled wave analysis (RCWA), also known as the Fourier modal method (FMM). The method is heavier computationally, but does not have the height limitations of the Rayleigh method. It is also better-suited for calculations with structures that have steep slopes.

The paper is organized as follows. The fabrication and characterization of the samples are described in Section 2. In Section 3, we present the expressions of the effective medium theories considered and the consequences of considering the structured layer as a homogeneous film for the calculation of the reflectivity. In Section 4 we briefly describe the two rigorous approaches to the calculation of the reflectivity that we have mentioned, namely the Rayleigh and the Fourier modal methods. The results are presented in Section 5, together with a discussion and, finally, in Section 6 we present our conclusions.

2. Nanostructured silicon samples

To explore the effective medium properties of nanostructured silicon layers at telecommunication wavelengths, we decided to focus on systems consisting of *circular* silicon nanopillars of a given radius that were arranged in an ordered or disordered fashion over the surface of the silicon substrate.

The fabrication of the samples started with 500 μm-thick, 1×1 cm^2 substrates of bulk silicon. The substrates were cleaned by immersing them in an ultrasonic bath of acetone for 15 min. They were then rinsed in isopropanol, blow-dried under a nitrogen flux, baked on a hot plate at 300 °C for 15 min, and allowed to cool and stabilize overnight. The cleaned substrates were spin-coated with a primer layer of hexamethyldisilazane (HMDS), and a 200 nm layer of a negative electron resist (ma-N 2400). After baking them for two minutes at 80 °C, the samples were coated with a layer of ESpacer 300Z, to prevent charging effects during the exposure. Then, the samples were rinsed with deionised water and dried.

The electron beam lithography (EBL) was carried out in a region of 1×1 mm^2 using a Raith system with a dose of 26 μC/cm^2. To design the exposure pattern, we first generated a "geometry matrix", consisting of ones and zeroes, that represents a top view of the desired geometry. The ones correspond to the silicon pillars and the zeroes to the region that will be etched at a later stage. The intended radius of the circular nanopillars was 75 nm. After exposure, all samples were developed in a solution made by combining equal quantities of ma-D 525 developer and deionised water for 60 s, rinsed in deionised water for another three minutes, and blow-dried under a nitrogen flux. Following the development, the samples were baked in an oven at 100 °C for ten minutes. An example of a periodic sample after the lithographic process is shown in Fig. 1(a). We point out that with negative resits, it is the exposed areas that remain on the surface of the substrate after development.

In the reactive ion etching (RIE) process, a plasma is generated by ionizing gas molecules in a low pressure chamber. The high-energy ions from the plasma attack the silicon on the wafer surface and remove material. To create the silicon pillars in our samples, the samples were subjected to a RIE process in a Plassys MEB400 using O_2 and SF_6 at 2×10^{-5} Torr and 90 W for three minutes in the first step, and O_2 with the same parameters for one minute in the second step. The height of the pillars is controlled by the time of etching. An example of the result is shown in Fig. 1(b).

Two types of samples were produced by this method. The first was a *periodic* structure, referred to as Sample A, in which the pillars formed a square lattice of period $a = 450\ nm$. In the second sample (Sample B), the pillars were placed in *random* positions with a pillar density that is equal to that in the periodic sample. This was achieved by choosing the exposure area and the total number of pillars to have the same values that we have in the periodic sample; that is, the exposure area was 1×1 mm^2 and the number of pillars was $\mathcal{M} = (2222)^2$. The positions of the pillars were decided through the following procedure: The exposure area was divided into a square lattice of equally spaced intervals of the same size as the pillar diameter (which happens to be one-third of the period). Then, two uncorrelated random integers ξ_1 and ξ_2 were drawn from a uniform distribution on the interval $[1, \mathcal{N}]$, where $\mathcal{N} = 6666$ is the number of cells in each direction of the lattice. If the cell labeled (ξ_1, ξ_2) was not occupied and nor were its nearest neighbors, then a pillar was placed at the center of the cell (ξ_1, ξ_2). This procedure was repeated until the number of pillars placed equaled $\mathcal{M}$. Note that for samples produced in this way the minimum center-to-center separation between neighboring pillars is two pillar diameters (or 300 nm for the radius assumed here).

Figs. 1 and 2 present SEM images of Samples A and B, respectively. One observes that the fabricated nanopillars have a lager cross section area at the base than at the top [Fig. 1(b)]. By analyzing SEM images of Sample A, both those in Fig. 1 and other SEM images taken of the same sample, it was found that the pillars have a shape that can be approximated by a truncated cone with approximate top and base radii $\rho_t = 85 \pm 5\ nm$ and $\rho_b = 105 \pm 10\ nm$, respectively. The structure was measured to have a nominal period of $a = 450 \pm 5\ nm$. The height of the pillars was found to be $\zeta_0 = 190 \pm 5\ nm$. It should be mentioned that due to the discretization of the ideal positions, Sample A showed some undesired features; the distance between pillars ended up having periodic variations and the cross section of the pillars was not quite circular. These issues are illustrated in the SEM image presented in Fig. 1(a).

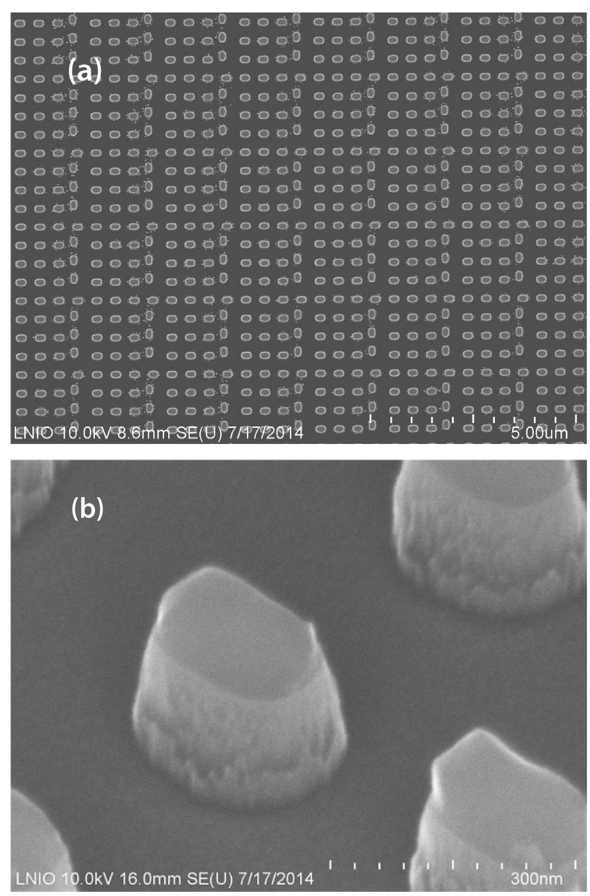

Fig. 1. SEM images of the periodic sample (Sample A) showing: (a) a large scale view of the structure after the lithography process but before etching; and (b) a detailed view of the nanopillars after etching.