Nontrivial optical response of silicon triangular prisms

M Poleva1, K V Baryshnikova1, K Frizyuk1, and A B Evlyukhin2,1
1The Faculty of Physics, ITMO University, St. Petersburg 197101, Russia
2Leibniz Universitat Hannover, Hannover 30167, Germany

Abstract. The electromagnetic response of silicon triangle nanoprisms in the near-infrared region is investigated. It is revealed that the bianisotropic dipole approximation is insufficient for this geometry since the direct application of the Onsager-Casimir symmetry rule to the dipole response leads to a contradictory conclusion. We show that to resolve this contradiction, it is necessary to take into account the nonlocal contributions of higher orders to the excited electric and magnetic dipole moments of the prisms. However, the inclusion in the consideration of nonlocal corrections to the dipole moments leads to the need to take into account the excitation of multipoles of a higher order than dipoles.

1. Introduction
These days the key target of researchers in the field of modern technology is to increase the speed of transmitting and processing the information and the computational capacity. Since most of the devices work via electrical impulses, they possess severe limitations due to the finite mass and non-zero charge of the electron. A possible solution to overcome these difficulties is the usage of photons instead of electrons as the main data carriers. The science that investigates the interaction of light with nanostructures, which such devices consist of, is called nanophotonics [1, 2, 3].

Usually, nanostructures are based on the numbers of so-called meta-atoms – specific elements, from which the whole structure is constructed of. The properties of nanostructure depend both on the features of each meta-atom and their relative positions. If cumulative effects are not excited in the structure, the properties of each meta-atom (the size, the shape and the material) play a major role. That is why the investigation of individual nanoparticles and their clusters is of so high interest to the nanophotonics community [4]. To explain, manage and predict optical properties of nanoparticles several methods were proposed, including CDA (coupled dipole approximation) method [5]. It shows their high applicability to a lot of different nanophotonics tasks. However, the last researches show that some scattering effects could not be explained with this approximation, and need to take into account the high order multipoles [6] or non-local response [7]. It was shown that in the general case, the electric response of the nanoparticle can be associated with both electrical and magnetic component of the incident field and their derivatives, and vice versa, the magnetic response is not only with magnetic, but also electric field and their derivatives [8]. In this work, we consider a very specific case of light interaction with a single prismatic shaped dielectric building block with the equilateral triangle at the base and show that it requires explanation with both non-local and high-order multipoles consideration.
2. Results and Discussion

To investigate the electromagnetic response of the prismatic shaped dielectric particle with the equilateral triangle at the base we considered a dipole bianisotropic approximation, i.e. the electric and magnetic dipole moments are determined only by the incident fields in a certain point (ordinary this point corresponds to the particle centre of mass). The location of the particle in respect to the coordinate axes is shown in Fig. 1(a). In order to realize the dipole resonances in the near-infrared range we chose the following parameters for modelling in COMSOL Multiphysics™ simulation software: radius of the circumscribed circle of the base triangle is \( R = 300 \) nm, height along the \( z \)-axis is \( h = 188 \) nm, the scatter material is silicon, for the surrounding medium \( \varepsilon_d = 1 \) and \( \mu_d = 1 \), the operating wavelength range is 900-1200 nm. In this range, for crystalline silicon, we can assume the dielectric constant to be \( \varepsilon_p = 12.67 \). To make sure that the usage of the dipole approximation is accurate we evaluated scattering cross-section and multipole decomposition for both lateral and normal incidence using exact formulas from [9, 10]. In Fig. 1(b,c), we see that the quadrupole contributions to the total cross-section are significantly smaller than the dipole ones and the quadrupole response can be neglected. Hence, we assume that only bianisotropic dipole approximation is sufficient for our study. Later, we will show, why this assumption may be failed.

In bianisotropic dipole approximation the local electromagnetic response can be described with the following relations [11]:

\[
\begin{align*}
p &= \alpha^{EE} D_{in} + c_d^{-1} \alpha^{EH} H_{in} \\
m &= \alpha^{HH} H_{in} + c_d \alpha^{HE} D_{in},
\end{align*}
\]
where $p$ and $m$ are the electric and magnetic dipole moments, respectively, excited by the electric displacement $D_{in}$ and magnetic $H_{in}$ incident fields, $c_d$ is the speed of light in the ambient space, $\alpha^{EE}, \alpha^{EH}, \alpha^{HE}, \alpha^{HH}$ are the $3 \times 3$ blocks of polarizability tensor $\alpha$, and each one of them represents a part of the dipole response to the incident fields. Since we consider the system without external time-odd bias field or external time modulation, i.e. reciprocal system, these blocks obey the Onsager-Casimir symmetry relations, which follow from the time-reversal symmetry of Maxwell’s equations [11, 8]:

$$\alpha^{EE} = (\alpha^{EE})^T, \quad \alpha^{HH} = (\alpha^{HH})^T, \quad \alpha^{EH} = -(\alpha^{HE})^T$$  \hspace{1cm} (2)

Assuming that the dipole approximation (1) is valid for the prism with the equilateral triangle at the base, we check that symmetry rules (2) are satisfied using the approach presented in [12]. First, we calculate the electric dipole moments excited by external $x$-polarized plane wave propagating firstly from $z$ and then $-z$ directions. As shown in Fig. 2(a), the electric dipole excites only in the direction of the incident electric field, i.e. oscillates along $x$-axis. For both incident directions with saving the polarization, the electric dipoles have the same absolute values and signs, which means that they are excited only by the incident electric field (since wave vector, electric and magnetic fields of the incident wave form the right-handed system, if we keep the direction of the electric field amplitude but rotate the wave vector by $180^\circ$.

![Figure 2](image-url)
degrees, the direction of the magnetic field amplitude will be also rotated by 180° degrees, and the sign of magnetic field changes). In this case from Eqs. (1), we conclude that $\alpha_{zy}^{EH} = 0$. Hence, from (2), it is followed that $\alpha_{yz}^{HE} = 0$ as well. However, in Fig. 2(b), it is revealed that z-polarized wave from y-direction excites the magnetic dipole not only in the incident magnetic field x-direction but also in the incidence y-direction. Moreover, the magnetic dipoles oscillating along the incidence direction for both $k_y$ and $-k_y$ have the same values and signs, which is shown in Fig. 2(c). This means that they are excited by the incident electric field, and $\alpha_{yz}^{HE} \neq 0$ for these irradiation conditions. Consequently, in the framework of the bianisotropic dipole approximation, we received a contradiction, which is as follows: on the one hand, from numerical calculations we obtained that $\alpha_{zy}^{EH} = 0$ and $\alpha_{yz}^{HE} \neq 0$, on the other hand, applying the Onsager-Casimir relations (2), we have $\alpha_{zy}^{EH} = -\alpha_{yz}^{HE}$. The last relation follows from the reciprocity property of the system with the triangular prism. Therefore, to resolve this contradiction we have to conclude that the bianisotropic dipole model (1) is not sufficient. To explain the phenomenon of dipoles exciting in the incidence direction we need to consider higher-order nonlocal contributions to the dipole moments stemmed from space derivatives of the incident fields. However, the inclusion in the consideration of nonlocal corrections to the dipole moments inevitably leads to the need to take into account the excitation of multipoles of a higher order than dipoles [8, 7].

3. Conclusion
It is been revealed that the bianisotropic dipole approximation is not sufficient to analyse the electromagnetic response of the considered dielectric prisms with the equilateral triangle at the base. Description of their dipole response must include nonlocal corrections higher than the bianisotropic terms. For an explanation of this feature, one can apply the symmetry theory and modal analysis. Our further investigations will be based on these approaches.

4. Acknowledgments
The work was supported by the Russian Science Foundation (project No. 21-72-20184).

References
[1] Krasnok A, Makarov S, Petrov M, Savelev R, Belov P and Kivshar Y 2015 Metamaterials X vol 9502 (International Society for Optics and Photonics) p 950203
[2] Evlyukhin A B, Tuz V R, Volkov V S and Chichkov B N 2020 Phys. Rev. B 101 205415
[3] Zheludev N I and Kivshar Y S 2012 Nat. Mater. 11 917–924 ISSN 1476-4660
[4] Terekhov P D, Baryshnikova K V, Artemyev Y A, Karabchevsky A, Shalin A S and Evlyukhin A B 2017 Physical Review B 96 035443
[5] Evlyukhin A B, Reinhardt C, Seidel A, Luk’yanchuk B S and Chichkov B N 2010 Physical Review B 82 045404
[6] Shamkhi H K, Baryshnikova K V, Sayanskiy A, Kapitanova P, Terekhov P D, Belov P, Karabchevsky A, Evlyukhin A B, Kivshar Y and Shalin A S 2019 Physical review letters 122 193905
[7] Bobylev D A, Smirnova D A and Gorlach M A 2020 Physical Review B 102 115110
[8] Achouri K and Martin O J F 2021 arXiv:2102.08197 (Preprint 2102.08197) URL https://arxiv.org/abs/2102.08197v1
[9] Alaee R, Rockstuhl C and Fernandez-Corbaton I 2018 Opt. Commun. 407 17–21 ISSN 0030-4018
[10] Evlyukhin A B and Chichkov B N 2019 Phys. Rev. B 100 125415 ISSN 2469-9969
[11] Asadchy V S, Diaz-Rubio A and Tretyakov S A 2018 Nanophotonics 7 1069–1094 ISSN 2192-8614
[12] Asadchy V S, Fanaiyev I A, Ra’dì Y and Tretyakov S A 2014 Photonics Nanostruct. Fundam. Appl. 12 298–304 ISSN 1569-4410