Analysis of terahertz wave nonlinear reflection by an array of double silicon elements placed on a metal substrate

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Abstract
We demonstrate simulation results of nonlinear reflection of intensive terahertz radiation from a silicon-on-metal metasurface involving an excitation of a high-Q trapped mode resonance. Conditions are presented to observe the effects of bistability and hysteresis of nonlinear reflection.

Keywords: periodic structure, reflective metasurface, localized field, resonance

1. Introduction

Modern optics technologies open an opportunity to produce resonant selectively reflecting metasurfaces. A metasurface is a planar patterned metal-dielectric or all-dielectric layer placed on a metal substrate. Thickness of a metasurface is usually very small in comparison with an electromagnetic field wavelength in a free space. However, the periodic patterning of a structure provides conditions for excitation of different types of resonances. A spectacular metasurface response manifests in resonance reflectivity and absorption, in electromagnetic radiation enhancement when using laser media, in exotic electromagnetic field boundary values, which may be the same as on a surface of an artificial magnetic wall, and in confinement of the intensive electromagnetic field inside the structure. Wavelength resonant selectivity of metasurface reflection is important in applications related to highly sensitive detection [1–3], particularly biological materials.

Metasurfaces confine the intensive electromagnetic field which is an important feature for the design of light controllable devices [4, 5] using nonlinear properties of materials. Modern laser-based sources provide power optical and terahertz radiation that can drive nonlinear properties of media [6].

Investigations of metasurfaces are frequently performed using semiconductors as nonlinear constitutive materials. In many cases, silicon is preferable in terahertz frequency range. For instance, in condensed matter physics investigations, a silicon anti-reflection coating has been involved and designed for planar metamaterials enhancing an electromagnetic terahertz field of pumping to prevent a probing light reflection by metallic elements of the metamaterial [7]. Results of experimental research on nonlinear properties of silicon wafer with metallic periodical structure placed on one of its surfaces are presented in [8].

The main factor defining spectacular properties of a metasurface is a resonant interaction of electromagnetic waves with a patterned metallic or dielectric layer. A special design of a metasurface unit cell can provide us an opportunity to excite high-Q resonances of trapped mode type [9–11]. A more intensive inner electromagnetic field is the main difference of a trapped mode resonance from usual types of resonances.

Nonlinear media may be included in the device as some elements of the patterned structure which constitutive parameters have dependence on the field intensity. Bistability and hysteresis are the feature effects of the reflection by a nonlinear metasurface. Due to these effects nonlinear resonant reflecting metasurfaces are quite promised for application as...
modulators, limiters, switches and other devices of the terahertz frequency range [12].

Thus, in this paper we for the first time demonstrate a numerical simulation of nonlinear reflection of intense terahertz radiation by the silicon-on-metal metasurface involving an excitation of a high-Q trapped mode resonance.

2. Reflective array design and theoretical methods

A square unit cell of the proposed reflective periodic metasurface is shown in the insert of figure 1. The structure is an array of silicon bars, which are placed on a metallic substrate (a copper foil). The array is periodic in two directions 0x and 0y. Each unit cell contains two silicon bars of the same thickness and length, but of different widths. We have chosen such asymmetric unit cell of the metasurface to provide an excitation of the high-Q trapped mode resonance [10]. The array periodicity along 0x and 0y axes is \( L = 205 \text{ mkm} \). The length of the bars is 195 mkm. The bars with widths of 50 mkm and 123 mkm are located at a distance of 16 mkm from each other. The thickness of the bars and copper foil is 35 mkm and 100 mkm, respectively. In potential applications, a metal substrate is envisaged as a good heat removed constructive element, reducing the time of response on a control variation of incident wave intensity.

For the simulation of the array spectral reflectivity in a linear regime the rigorous numerical-analytical method and the developed computer code were used. They are based on volumetric integral equations of macroscopic electrodynamics for solving problems of electromagnetic wave scattering by planar multilayer magnetodielectric structures which are periodic in two directions along their plane [13, 14]. In this approach the electromagnetic field at some point is the sum of the incident wave field and the field scattered by the structure. This presentation for the field is converted into integral equations for the equivalent electric and magnetic polarization currents if the observation point is inside the scattering structure. Discretizing the integral equations and using the double Floquet–Fourier series expansion we obtain a set of integro-differential equations in integral functionals related to the polarization currents in the small parallelepiped segments that the plane unit cell is partitioned on. The equivalent electric and magnetic polarization currents in each segment having number \( i \) along the 0x axis and \( j \) along the 0y axis with corresponding permittivity and permeability are related to the electric and magnetic fields in it as follows:

\[
\begin{align*}
J^e_{ij}(x, y, z) &= (\epsilon_{ij} - 1)E^e_{ij}(x, y, z), \\
J^m_{ij}(x, y, z) &= (\mu_{ij} - 1)H^m_{ij}(x, y, z).
\end{align*}
\] (1)

Then, given a solution for the integral functionals a scattered field outside the structure can be calculated. A form of the periodic cell and the values of dielectric permittivity of the structure materials are not limited in the framework of the method. Dielectric permittivity can be complex; its imaginary part can be positive or negative, i.e. the field absorption and amplification are taken into account in the solving procedure.

The developed numerical code has been tested for a large number of scattering problems and a comparison with results of different commercial codes and measurements has been made. The tests manifested an excellent accuracy of the developed code and convenience in applied problems of electromagnetism, among them the study of transmission through sub-wavelength holes in plasmonic structures [15], guided-mode resonances [16], electromagnetic field interaction with 3D lattice dielectric structures involved a defect layer and gain material [17, 18].

In the nonlinear regime, for relative dielectric permittivity we assume Kerr’s dependence on the electric field intensity. We use the approximation of monochromatic waves and study the spectral properties of this reflecting metasurface at normal incidence of a plane x-polarized electromagnetic wave impinging from the z < 0 semi-space. The base of numerical code includes the previously mentioned method of volumetric integral equations of macroscopic electrodynamics which was combined with a set of two transcendental equations on the field intensity in the middle points of each bar of the unit cell. The solution of this equation set was used to determine an actual value of the relative permittivity of the bars. The numerical solution of the set was found by the method of simple iterations with using a relaxation.

In the simulations, the results of which are presented here, we assume the relative dielectric permittivity of n-type silicon of bars \( \epsilon = \epsilon_0 + \chi(3)E^2 \) where \( \epsilon_0 = 11.70 - i0.01 \) that is, the electromagnetic material losses were taken into account, the third-order nonlinear susceptibility is \( \chi(3) = 3.5 \times 10^{-8} \) esu [19], and the relative permeability is \( \mu = 1 \). For the dielectric permittivity of the substrate the reference book data [20] for copper in the terahertz frequency range was used \( \epsilon_e = -13700 - i159000 \).

At each iteration step electric polarization currents used in the solution algorithm are presented through dielectric permittivity values, obtained at a previous step. As an initial approximation, dielectric permittivity for the linear problem (1) are used \( \chi(3) = 0 \).

In this paper, as mentioned previously, we assume that the dielectric permittivity of nonlinear material of the bars changes according to the electric field intensity value in the central point of each bar. The system of two nonlinear equations takes the form

\[
\begin{align*}
I_1 &= f(E_{inc}, \omega, \epsilon_0 + \chi(3)I_1, \epsilon_l + \chi(3)I_2) \\
I_2 &= f(E_{inc}, \omega, \epsilon_0 + \chi(3)I_1, \epsilon_l + \chi(3)I_2),
\end{align*}
\] (2)

where \( I_1 = E_1E_1^*, I_2 = E_2E_2^* \), \( E_1 \) and \( E_2 \) are electric field strengths in the bar centers, \( E_{inc} \) is a strength of the incident electric field, \( \omega \) is a frequency. The function \( f \) means the solution algorithm and computer code gives us scattering characteristics and electromagnetic field values in the structure.

Using expressions (2) we consider an iterative method as follows
where $\tau$ is a constant relaxation parameter. In the simulations, we have used the values $\tau = 1; 2; 2.5; 3$ defined as a result of numerical experiments for solution convergence.

3. Linear reflection regime of the metasurface

The proposed controllable metasurface has a set of sharp resonances clearly manifested as maxims of absorption in the terahertz range of frequencies. The simulation results of electromagnetic wave reflection by the investigated structure are plotted versus normalized frequency in figure 1. The term ‘normalized frequency’ $L/\lambda$ ($\lambda$ is a wavelength in free space) is of frequent use in the theory of wave diffraction. On the upper abscissa axis, the corresponding frequency in THz is presented. It is noticeable that in the case of the bars of different widths there are additional resonances on the reflectance characteristic that are not presented in the spectrum of the symmetric structure and the structure with one bar per unit cell.

In order to study the physical origin of resonance behavior of the metasurface characteristics, numerical simulations were made and maps of the internal fields in the studied structure were built. In this way, we reveal patterns of the field distributions and places of greatest confinement of electromagnetic power at the resonance conditions.

The first low-frequency and low-Q resonance (figure 1, lines 1–4) is due to the electromagnetic field formation typical of a magnetic dipole parallel to the $0_y$ axis with a maximal magnetic field in the wider bar and a maximal electric field between end faces of the wider bars of neighbored unit cells. The electric and magnetic fields reach 23 and 175 conventional units, respectively. In the linear regime, we assume electric field strength of the incident wave to be unity.
In conditions of the second high-Q resonance next in direction of increasing frequency (figure 1, line 1) we have observed opposite electric dipoles along each bar, parallel to the $0x$ axis. The greatest values of electric and magnetic fields in the narrow bar are respectively 63 and 830 conventional units. This resonance is the most promising one for the investigation of nonlinear response and applications due to its high-quality factor and such field distribution along the unit cell that a maximum of the electric field intensity is inside of the bars. These two conditions provide advantageous opportunities for an electromagnetic field coupling with the nonlinear silicon of bars. The peculiarity of the resonance is associated with excitation of a trapped mode field distribution inside the unit cell. The resonance normalized frequency $L/\lambda$ is 0.6426.

Next, the third resonance (figure 1, line 1) is accompanied by appearance of two magnetic dipoles parallel to the $0y$ axis in each bar and oppositely directed in the wide and narrow bars. The concentration of electric and magnetic fields reaches respectively 60 and 390 conventional units.

If there is a need to see complete field maps for the set of resonances and reveal the origin of each resonance, you can refer to the paper [3]. In this paper, the first seven resonances...
lowest on the frequency were studied in detail including the resonant field distribution in the unit cell of a structure very similar to the metasurface being under our investigation here.

Thus, in the following, we will study a nonlinear reflection by the metasurface with two different bars in an unit cell at frequencies close to the resonance normalized frequency $L/\lambda = 0.6426$.

### 4. Nonlinear reflection regime

In the nonlinear reflection regime, the intensity of an incident electromagnetic field is large enough to produce heating inside the lossy resonant metasurface that can essentially modify the permittivity of silicon bars. The effect may be interpreted as a third-order Kerr nonlinearity [21]. As a result, the structure reflectivity depends on the incident wave amplitude and may be controllable. At a frequency close to the trapped mode resonance in the linear regime, we can observe sharp variations in dependencies of the reflection coefficient on the incident field strength $E_{\text{inc}}$, as shown in figures 2 and 3.

At frequencies higher than the resonance frequency of linear reflection, the increase in the incident wave amplitude leads to the resonance destroying and to monotonic increasing of the reflection coefficient (see figure 2, lines marked by letters B and C). We observe more interesting behavior of the reflection coefficient at frequencies below the resonance frequency of the linear regime (see figure 2, lines marked by letters a, b, c and d and also figure 3). The lower is the frequency the more is the electric field strength of the incident wave $E_{\text{inc}}$ which corresponds to the resonance. Moreover, the metasurface reflection manifests bistability and hysteresis in dependence on $E_{\text{inc}}$.

Bistability is a manifestation of an electromagnetic field self-action in the nonlinear metasurface under consideration with a feedback, in which two possible stationary states of a reflected wave field correspond to a certain intensity of the incident radiation. Manifesting a hysteresis property, the amplitude of the reflected wave can take one of two values. With a cyclical change in the incident wave intensity over a wide range, the metasurface with bistable reflection operates

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**Figure 4.** Dependencies of frequencies of sharp resonant increase and decrease in the reflection coefficient on the incident field strength.

**Figure 5.** Variation of a permittivity and $E_{\text{inc}}$ in the central point of each bar for the relative frequency $L/\lambda = 0.6380$ with the incident field strength. Labels 1 and 2 mark the narrow and wide bars respectively.
reversibly, and the previous state of the reflection uniquely determines which of the two stable field states is realized in the reflected field.

Occurrence of a region of an incident radiation intensity values, where the reflection coefficient is double-valued, is caused by the feedback in the nonlinear system under study.

In figure 4, we present dependencies of resonant frequencies of abrupt increase and decrease of the reflection coefficient on the strength of the incident field. The hysteresis range begins from the strength approximately equal to 200 statvolt/cm. A distance on the abscissa axis between the plot branches corresponds to a width of the hysteresis loop (see figure 3) for frequencies on the ordinate axis.

In a strong resonant field inside the structure, permittivity of the semiconductor bars varies with the incident wave intensity. We have studied this variation of the permittivity frequencies on the ordinate axis. A distance on the abscissa axis between the plot branches corresponds to a width of the hysteresis loop (see figure 3) for strengths approximately equal to 200 statvolt/cm.

5. Conclusion

A nonlinear reflection of intensive terahertz radiation by the silicon-on-metal metasurface has been studied by numerical simulation. By involving an excitation of the high-Q trapped mode resonance, an essential enhancement of electric field near 1 THz.

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References

[1] Wang B-X, Zhai X, Wang G-Z, Huang W-Q and Wang L-L 2015 A novel dual-band terahertz metamaterial absorber for a sensor application J. Appl. Phys. 117 014504
[2] Yahiaoui R, Tan S, Cong L, Singh R, Yan F and Zhang W 2015 Multispectral terahertz sensing with highly flexible ultrathin metamaterial absorber J. Appl. Phys. 118 083103
[3] Sydorchuk N and Prosvirnin S 2017 Analysis of terahertz wave reflection by an array of double dielectric elements placed on a reflective substrate 22nd Int. Seminar/Workshop on Direct and Inverse Problems of Electromagnetic and Acoustic Wave Theory (Dnipro, Ukraine) pp 58–63
[4] Boyd R W 2008 Nonlinear Optics 3rd edn (New York: Academic)
[5] Keiser G R, Fan K, Zhang X and Averitt R D 2013 Towards dynamic, tunable, and nonlinear metamaterials via near field interactions: a review J. Infrared Millim. Terahz Waves 34 709–23
[6] Hoffmann M C and Fülöp J A 2011 Intense ultrashort terahertz pulses: generation and applications J. Phys. D: Appl. Phys. 44 083001
[7] Pancaldi M, Freeman R, Hudl M, Hoffmann M C, Urazhdin S, Vavassori P and Bonetti S 2018 Anti-reflection coating design for metallic terahertz meta-materials Opt. Express 26 2917–27
[8] Al-Naib I, Sharma G, Dignam M M, Hafez H, Ibrahim A, Cooke D G, Ozaki T and Morandotti R 2013 Effect of local field enhancement on the nonlinear terahertz response of a silicon-based metamaterial Phys. Rev. B 88 195203
[9] Khardikov V V, Iarko E O and Prosvirnin S L 2010 Trapping of light by metal arrays J. Opt. 12 045102
[10] Khardikov V V, Iarko E O and Prosvirnin S L 2012 A giant red shift and enhancement of the light confinement in a planar array of dielectric bars J. Opt. 14 035103
[11] Zhang J, MacDonald K F and Zheludev N 2013 Near-infrared trapped mode magnetic resonance in an all-dielectric metamaterial Opt. Express 21 26721–8
[12] Carretero-Palacios S, Minovich A, Neshov D N, Kivshar Y S, Garcia-Vidal F J, Martin-Moreno L and Rodrigo S G 2010 Optical switching in metal-slit arrays on nonlinear dielectric substrates Opt. Lett. 35 4211–3
[13] Yachin V V and Ryzanitseva N V 1999 The scattering of electromagnetic waves by rectangular-cell double-periodic magnetodielectric gratings Microw. Opt. Technol. Lett. 23 177–83
[14] Sydorchuk N 2008 Resonant wave scattering by plane periodic structures bounded by two homogeneous media Radio Phys. Radio Astron. 13 250–62 (in Russian)
[15] Sydorchuk N 2007 Transmission of optical and terahertz radiation through subwavelength hole arrays 12th Int. Seminar/Workshop on Direct and Inverse Problems of Electromagnetic and Acoustic Wave Theory (IEEE) pp 170–3
[16] Sydorchuk N 2008 Theoretical study of guided-mode resonances in planar doubly-periodic dielectric structures 12th Int. Conf. on Mathematical Methods in Electromagnetic Theory (IEEE) pp 538–40
[17] Sydorchuk N 2013 Analysis of electromagnetic wave interaction with quantum-dot gain material in 3D photonic crystals Int. Kharkiv Symp. on Physics and Engineering of Microwaves, Millimeter and Submillimeter Waves (IEEE) pp 204–6
[18] Sydorchuk N 2016 Electromagnetic properties of dielectric multilayer periodic structures with inclusions of gain medium 9th Int. Kharkiv Symp. on Physics and Engineering of Microwaves, Millimeter and Submillimeter Waves (IEEE) pp 1–4
[19] Narkowicz R, Siegrist M, Moreau P, Hogge J, Raguotis R and Gutierrez P 2017 Observation of ultrashort terahertz radiation from the far infrared to the x-ray region: Mg, Al, Cu, Ag, Au, Bi, C, and Al3O3 J. Opt. Soc. Am. B 34 739–44
[20] Makarov S V, Zalogina A S, Tajik M, Zuev D A, Rybin M V, Kuchmizhak A A, Juodkazis S and Kivshar Y V 2017 Light-induced tuning and reconfiguration of nanophotonic structures Laser Photonics Rev. 11 1700108