Bound states in the continuum in dielectric waveguides of finite size

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Abstract. We study bound states in the continuum related supercavity modes in finite lattices of silicon rods. Two low-frequency symmetry-protected modes are examined. We find that Q factor has almost cubic dependence on the rod number and 50 rods are enough for Q exceeds $10^4$. We discuss possible applications of these supercavity modes based on their electromagnetic field pattern. The structure surrounded by liquid media keeps its functionality by substitution silicon rods with rods made of Ge-Sb-Te.

1. Introduction

Recently bound states in the continuum (BIC) caught a lot of attention since in contrast to the electrons, photons are always in the continuum of the free space propagation modes [1]. BICs open attractive perspectives for trapping electromagnetic waves by a perfect resonator. For a system to support BIC with infinite quality (Q) factor the structure has to take an infinite parameter (size or permittivity), however practical systems can support supercavity modes which are BIC counterparts in finite samples [2].

Many applications of BIC were reported during the last decade. Supercavity modes acts as a feedback in a low threshold lasers [3]. Silicon metasurfaces integrated into a barcode device allows an imaging-based biosensor for fast and efficient determination of both concentration and structure of proteins [4, 5]. Optical tuning of silicon permittivity by high-speed laser pulses makes it possible to design switching device operating at terahertz frequencies [6].

Here we study a silicon-based structure designed for terahertz waves that allows analytical solution to the electromagnetic problem. Similar results take place for arbitrary operation frequencies after adjusting geometric sizes. For the case of liquid surrounding media (e.g. for biosensing) silicon can be substituted by material with higher permittivity to match dielectric index contrast. In particular, Ge-Sb-Te family of compounds are suitable materials for the middle infrared range [7, 8].

2. Results

We consider a one dimensional lattice of parallel infinite silicon rods forming a metasurface. Here we study the structure in a hundred micrometres size similar to the metasurface operating at terahertz frequencies reported recently [6], however owing to the scalability of the Maxwell’s equations a similar metasurface has same properties at any desired frequencies in the entire electromagnetic spectrum from the microwave to visible range. Our structures have the following
Figure 1. Schematic view of silicon metasurface. Infinite rods (along the $z$ axis) of radius $r$ and dielectric index $\varepsilon = 12$ are arranged in a lattice with period $a$. TE polarization is considered.

Figure 2. Spectra of periodic array of $N = 30$ silicon rods in the metasurface (a) and waveguide (b) regimes for in the TE polarization. The left inset in panel (a) shows details of the transmission spectra around the mode 1 for $N = 30$ (solid curve) and additionally for $N = 29$ (dashed curve); the arrows point to spectral features. The right inset in panel (a) shows details around the mode 1. Inset in panel (b) shows the Lorenz-Mie amplitudes for dipolar ($m = 0$, solid curve) and quadrupolar ($m = \pm 1$, dotted curve) multipoles of a silicon rod.

parameters. The lattice constant is $a = 300\ \mu m$, the rod radius is $r = 100\ \mu m$, silicon permittivity in the range of interest is approximately $\varepsilon = 12$, we examine structures with the rod number $N$ in the 10-to-100 interval. We study the TE polarized waves, that is the magnetic field oscillates along the rod axis $z$ (see figure 1).

The electromagnetic problem for the system described above has a rigorous solution by means of the multiple scattering theory. A set of non-overlapping rods having arbitrary radii and positions allows us to separate the problem into two logical parts. The first part is the scattering of an incident wave by each rod that can be obtained by the multipole expansion of the field around the rod centre and by applying Maxwell’s boundary condition (i.e., Mie theory). The second part is to re-expand scattered waves from one rod into the multipoles of incident field related to another rod. By combining these two parts we define a linear self-consistent equation that can be solved by algebraic methods. Details of the multiple scattering theory are described elsewhere (e.g. in [9]).
Figure 3. Magnetic field $H_z$ distribution of the two low-frequency supercavity modes of the periodic array of $N = 50$ silicon rods excited by a dipole source located near the left edge (shown by arrows): TE polarization. Red and blue colours correspond to positive and negative values of $H_z$, respectively. (a) The supercavity mode 1 at $f = 0.301$ THz; (b) the supercavity mode 2 at $f = 0.367$ THz.

For applications of realistic systems it is convenient to consider a metasurface configuration. A plane wave incidents from the normal direction to the structure. In our simulations the plane wave is approximated by a Gaussian beam with the waist covering the entire metasurface. To avoid effects of the field inhomogeneity in the vicinity of the rods transmission spectra are evaluated by integration of the electromagnetic energy passed through the structure over the line $4a$ in length located at the centre at the distance $2a$ behind the system. The spectra are normalized by a same integral evaluated for the free space with no rods. Figure 2a displays the transmission spectrum of the metasurface composed of $N = 30$ unit cells. For the mode analysis we also study our system in a waveguide regime. In this case the chain is excited by a two-dimensional point dipole source (that is a line emitter) located at one side with the distance $0.5a$ between the dipole and the centre of the outer rod. We obtain intensity spectra by similar integration procedure over the line of length $14a$ (along the chain) positioned symmetrically respective to the structure. The intensity spectrum of the $N = 30$ rods is demonstrated in figure 2b.

Intensity spectra in the waveguide configuration provide vast information about electromagnetic mode properties of our structure. Two propagation bands below 0.301 (band 1) and 0.367 THz (band 2) and two bandgaps are clearly seen in figure 2b. We notice that these frequencies correspond to those for the infinite systems ($N \to \infty$) 0.311 and 0.379 THz, respectively. The combs of intensive peaks are located at the high-frequency band edges. These peaks corresponds to standing waves with wave length $\lambda = 2l/n$, where $l$ is the chain length and $n$ is an integer mode number. We identify 8 peaks in the band 1 (and 7 in the band 2) which position demonstrates a quadratic dependence relative to the band edge, because of a quadratic dispersion of the bands near the $\Gamma$ point of the Brillouin zone. The transmission spectrum for the metasurface configuration in figure 2a exhibits less pronounce features corresponding to some peaks in the intensity spectrum in waveguide regime (figure 2b). In particular the transmission spectrum contains odd peaks of the band 2.

The mode profiles are shown in figure 3. There are the high-Q modes 1 and 2 with $n = 1$ which reveal different location of electromagnetic field. For the mode 1 at $f = 0.301$ THz the
field in each rod has dipole-like distribution. The intensity is predominantly localized inside the rods, however the hot spots spread above and below the metasurface. Neighbour rods oscillate in opposite phase. We notice that $f = 0.301$ THz matches well with the maximum of dipole response of silicon rods (see inset in figure 2b). The profile of mode 2 at $f = 0.367$ THz shows quadrupole-like field distribution in rods and neighbour rods oscillate in opposite phase as well. In this case the pattern exhibits hot-spot area between the rods and above and below the metasurface. Surprisingly enough this quadrupole-like mode has a remarkable shift off the maximum of quadrupole response of silicon rods at $f = 0.485$ THz (figure 2b).

The modes with odd number $n$ are modulated by cosine function along the structure and modes with even number $n$ are modulated by sine. The modes with $n = 1$ have the slowest envelope and in the limit of infinite rod number $N$ all rods have the same amplitude except the anti-phase condition for neighbour elements. In the metasurface plane the structure has the symmetry of the $C_{2v}$ point group. Modes with wave vector $k = 0$ being the $A$ representations orthogonal to plane waves that are the $B$ representations, therefore the $A$ modes are uncoupled of the free space and are the symmetry-protected BIC. The modes 1 and 2 studied here transform as the $A$ representations and because of finite $N$ they are high-Q supercavity modes. The symmetry protection is weakened due to the sine or cosine envelope, thus modes with higher $n$ have lower Q. Also we notice that the modes 1 and 2 have different parity. Hence, in the metasurface configuration the even Gaussian beam excites the even $n$ modes only in the band 1 modulated by sine and the odd $n$ modes only in the band 2 modulated by cosine. We notice that a plane wave with normal incidence excites mode 1 with $n = 1$, when the symmetry is effected by change of rod number (see inset in figure 2a for $N = 29$).

The size of metasurface is important for designing practical devises. We examine the Q factor of supercavity modes 1 and 2 as a function of the rod number. The peaks in spectra obtained in the wave guide configuration has negligible Fano asymmetry and we find the line width of modes with $n = 1$ by Lorentzian fitting. Q factor dependences are shown in the log-log scale in figure 4. It is clearly seen that all values are lain at a line uncovering that Q factor obeys the power law $Q \propto N^{\alpha}$. We notice that two supercavity modes have distinct $\alpha$, namely $\alpha_1 = 2.83$.
and $\alpha_2 = 3.25$ which are around the cubic dependence.

3. Conclusions

We have studied two high-Q supercavity modes supported by the periodic array of silicon rods. Q factor of these modes has been found to obey nearly the cubic dependence. The field pattern of mode 1 allows applications involving light-matter (rod material) interaction such as efficient harmonic generation and low-threshold lasing since the field is located in the rods. The field pattern of mode 2 with hot-spots between the rods enables sensing of molecules diluted in the surrounding media. For the case of liquid surrounding media with permittivity about 2 the rod permittivity has to be scaled up to 25-30 that is available for Ge-Sb-Te alloys in the mid IR range [7, 8]. Because of different imperfections of real samples typical limitation of Q factor is of orders $10^3$ - $10^4$. Therefore, size effects on supercavity mode Q factor are saturated at $N = 50$.

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