Resonant Scattering of Light by Finite Sparse Configurations of Silver Nanowires

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Abstract— **We consider the two-dimensional (2-D) scattering of the H-polarized plane wave by three discrete configurations made of periodically arranged circular cylindrical wires, using the field expansions in local coordinates and addition theorems for cylindrical functions. Resulting block-type matrix equation is cast to the Fredholm second-kind form that guarantees convergence of numerical solution. The scattering and absorption cross-sections and the near-field patterns are computed. The interplay of plasmon and grating-type resonances is studied for discrete arrays, corners and crosses made of nano-size silver wires in the visible range of wavelengths.**

Keywords-nanowire grating, scattering, plasmon resonance, grating resonance.

I. Introduction

Periodically structured scatterers, or finite-periodic gratings, arrays or chains of particles and holes in metallic screens (in 3-D) or wires and slots (in 2-D), are attracting large attention of researchers in today's nanophotonics [1-6]. This is caused by the effects of extraordinarily large reflection, transmission, emission, and near-field enhancement that have been found in the scattering of light by periodic scatterers. Recently it has been discovered that these phenomena are explained by the existence of so-called grating resonances or poles of the field function [3-6] (a.k.a. geometrical, lattice and Bragg resonances). Their wavelengths are just above the Rayleigh wavelengths [7], i.e. period being a multiple of the wavelength if all elementary scatterers of a grating are excited in the same phase and their size is a fraction of the period. In the wave scattering by infinite gratings, they lead to almost total reflection of the incident field by a thin-dielectric-wire grating in a narrow wavelength band [3,5].

Another type of resonances is observed for sub-wavelength noble-metal particles and wires in the mid-infrared and optical bands [8,9]. It is known that small material objects can exhibit resonance behavior at certain frequencies for which the object permittivity is negative and the free-space wavelength is large in comparison to object dimensions. The latter condition clearly suggests that these resonances are electrostatic in nature. Excitation of plasmons results in powerful enhancement of scattered and absorbed light that is used in the design of optical antennas and biochemical sensors for advanced applications. In the leading terms, the plasmon resonance wavelength depends on the noble-metal object shape but not on its dimensions. The goal of our paper is extension of this study to 2-D periodically structured silver-wire configurations of various shapes.

II. Scattering problem

Consider a finite collection of arbitrarily located M parallel wires illuminated by a plane wave as shown in Fig. 1. The wires are assumed to be identical infinite circular cylinders, each having radius a and complex relative dielectric permittivity ε. For a 2-D problem, one has to find a scalar function $H_z(\vec{r})$ that is the scattered-field z-component. It must satisfy the Helmholtz equation with corresponding wavenumbers inside and outside the cylinders, the tangential field components continuity conditions, the radiation condition, and the condition of the local power finiteness.

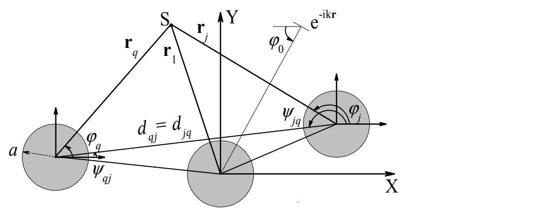

Figure. 1. Generic problem geometry and corresponding notations: a plane wave is incident on a finite number of identical parallel circular cylinders.

The full-wave numerical solution can be obtained, similarly to [10-12], by expanding the field function in terms of the azimuth exponents in the local polar coordinates (Fig. 1), using addition theorems for cylindrical functions, and applying the boundary conditions on the surface of each of M wires. This leads to an infinite $M \times M$ block-type matrix equation where each block is infinite. Still it is possible to see that the matrix equations used in the previous papers did not guarantee the convergence of numerical solutions. Here, we understand the convergence in mathematical sense, as a possibility of minimizing the error of computations by solving progressively larger matrices. (Frequently, convergence is mixed up with accuracy. Many divergent numerical schemes are able to provide a few first digits correctly however fail when a better accuracy is required.) We have also found that this defect of earlier publications can be easily fixed by re-scaling the unknown coefficients – see [5] for details.

The obtained in such a way matrix equation is a block-type

Fredholm second kind equation. In this case the solution of equation with each block truncated to finite order N converges to exact solution if $N \to \infty$, and quite rapidly. The results presented below were computed with $N = 4$-6; this provided 3 correct digits in the far-field characteristics of the sparse gratings of silver wires with radii $a \leq 75$ nm and periods $p \geq 200$ nm. Note that denser gratings need larger values of N to achieve the same accuracy.

We have considered three sparse ($\rho - 2a > a$) configurations of finite number of sub-wavelength silver nanowires: linear gratings (discrete line), discrete corners and discrete crosses. Dense configurations are also interesting objects however they deserve a separate study. To characterize far-field scattering properties of considered discrete scatterers, we have used the total scattering (TSCS) and absorption (ACS) cross section frequency dependences and calculated the field patterns in the near-field zone. In Figs. 2-4, the wavelength varies from 300 nm to 500 nm and the complex-valued dielectric function of silver has been borrowed from [13].

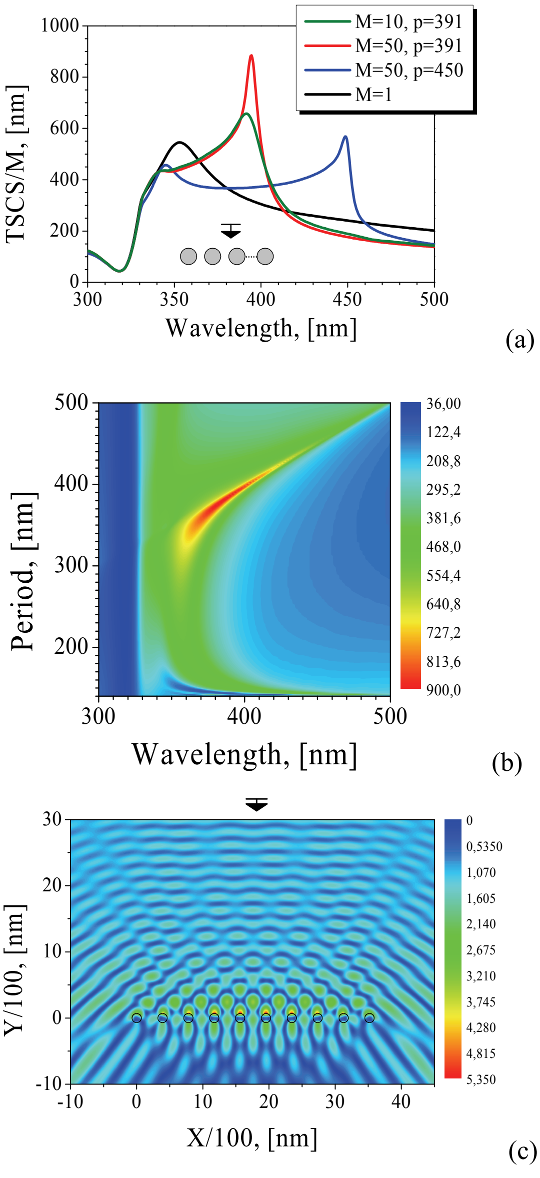

Figure 2. TSCS per wire as a function of wavelength (a) and as a function of wavelength and period (b), near-field amplitude pattern (c) for the H-wave incident broadside ($\varphi_0 = \pi/2$) on the gratings of $M = 50$ (a), (b) and $M = 10$ (c) silver nanowires with radii $a = 70$ nm.

III. Results and Discussion

A. Linear gratings

One of the important questions is what can be expected from the scatterer characteristics if the plasmon and the grating resonance wavelengths coincide. This can be achieved using the period of the wire grating as an instrument, because the plasmon resonance has almost fixed wavelength near to the single-wire value around 350 nm. For example, in Fig. 2(a) presented is the plot of the TSCS as a function of the wavelength for a stand-alone silver wire with radius 70 nm. It has broad maximum at 353 nm.

In Fig. 2(a), presented are also the plots of TSCS per wire as a function of the wavelength for several sparse gratings of $M = 50$ silver wires with radii 70 nm (at normal incidence). One can see that if the period is far from the plasmon resonance wavelength, the grating resonance has little effect on TSCS: it can be found to form a small spike on the red-side slope of plasmon resonance. This behavior changes dramatically, if two resonances are tuned nearer - in that case one can see a more intensive grating resonance. As visible, enhancement in TSCS can reach 1.7. The combined peak and hence the period should be red-shifted relatively to plasmon resonance of a single wire. As we have found, the optimal wire radii to observe the strongest TSCS enhancement lie in the range of 25 nm to 70 nm.

In Fig. 2(b), presented is a relief of per-wire TSCS (i.e. normalized by M) at normal incidence, as a function of two parameters: wavelength and period, for the gratings of 50 silver wires with the radii 70 nm. In this case one can see a sharp "ridge" stretching along the line $\lambda = p$ that marks the grating resonance. Another, broader ridge stands at the fixed wavelength near to 350 nm – this is plasmon resonance. The strongest enhancement of TSCS is found near to the junction of these two ridges, for periods slightly larger than the plasmon wavelength.

In Fig. 2(c), presented is the near-field amplitude pattern for the 10-wire sparse grating with $a = 70$ nm at the wavelength of the combined resonance. The field hot-spot maxima can be seen near the illuminated sides of the wires similarly to the single-wire case [8]. Besides of that one can clearly see two standing-wave patterns near to the grating: one is above the illuminated side – it is formed by the incident plane wave and the reflected field. Another is an "orthogonal" wave standing along the wires; it is formed by two oppositely propagating ±1-st quasi-Floquet harmonics of the grating as the wavelength near the value $\lambda = p$ (see [6] for details).

B. Discrete corners

Fig. 3 presents the results computed for discrete right corners made from silver wires with $a = 60$ nm. In Fig. 3(a),

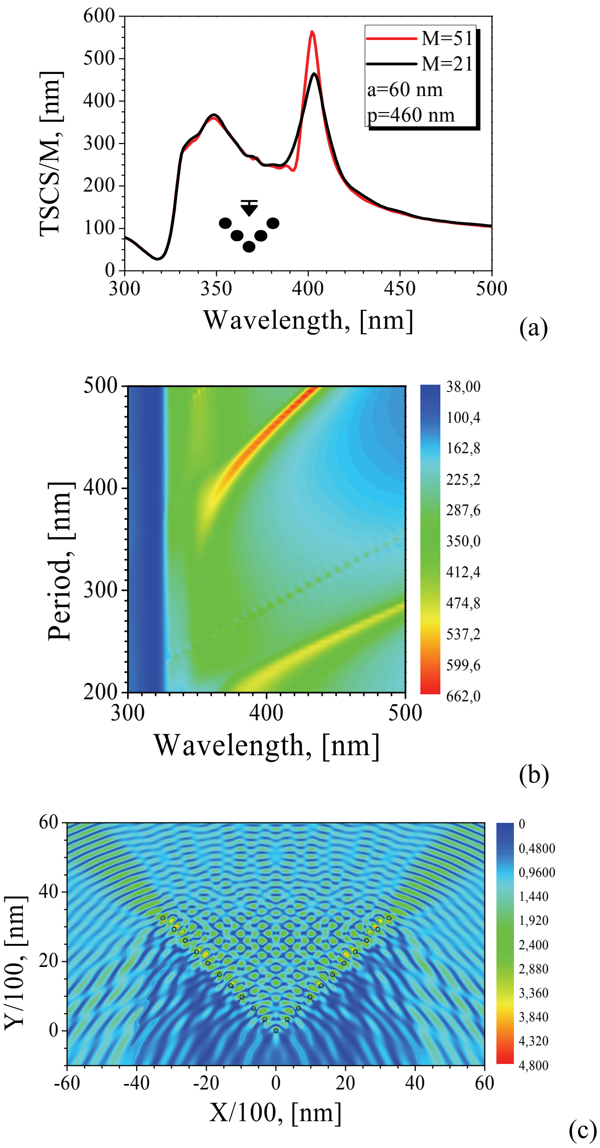

Figure 3. The same as in Fig. 2 for discrete right corners from silver nanowires with radii *a* = 60 nm.

presented are TSCSs per one wire as a function of the wavelength for discrete corners of 21 and 51 wires with period 460 nm. One can see two resonances in both cases. The first resonance is at the wavelength of 348 nm; this is the plasmon resonance which can be observed at the same location for a stand-alone wire. The second resonance is at the wavelengths of 403 nm and 402 nm for the 21 and 51-wire corners, respectively. This is the grating-type resonance because it becomes greater for larger *M*. Because of the chosen corner orientation, the wavelength of the grating resonance is shifted from the period value, corresponding to the Rayleigh value for the +2-nd Floquet harmonic grazing.

Our numerical simulations confirm that such a discrete corner can enhance the maximum values of TSCS per one wire at certain wavelengths. In Fig. 3(b), presented is a relief of TSCS as a function of two parameters: wavelength and period for discrete right corners made of 51 silver wires. On this relief, one can see two areas of high TSCS values. They stretch along the "ridges" corresponding to the grating resonances associated with the +2-nd and +1-st Floquet harmonics in the grazing regimes.

In Fig. 3(c), presented is the near-field pattern for a discrete corner made of 21 silver wires at the grating-resonance wavelength of 403 nm. This configuration has the incident wave coming from the internal side of the corner along the symmetry axis. One can see several "hot spots" near the wires from the illuminated side of the corner rays. Overall field pattern is a superposition of several scattered quasi-plane waves in this grating resonance.

C. *Discrete crosses*

The configurations where the grating-type resonances are well developed imply large *M* as the corresponding Q-factors grow up with larger *M*. Therefore we have studied the cross-shape scatterers with *M* up to 101 wires in four arms of cross,

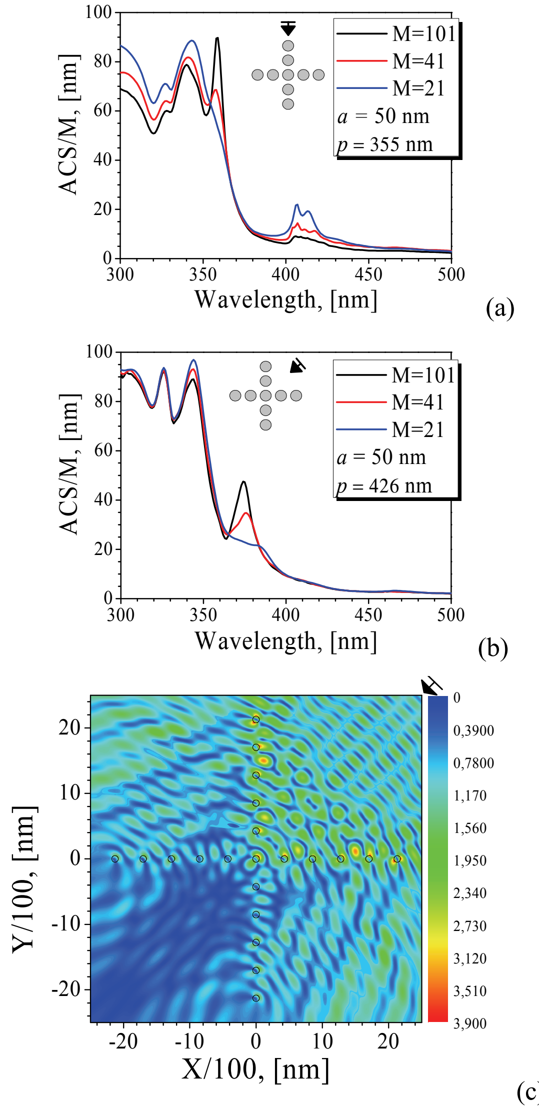

Figure 4. ACS per wire as a function of wavelength (a),(b) and near-field pattern (c) for the H-wave incident normally (a) and under the angle $\varphi_0 = \pi/4$ (b),(c) on the crosses of silver nanowires with radii *a* = 50 nm.

i.e. with one central wire and four 20-wire arms.

In Figs. 4(a),(b), we present the spectra of per-wire ACS for the cross-shaped periodic scatterers with radii of each wire 50 nm, in the visible range, under two variants of the H-polarized plane wave incidence: along a cross arm and along a diagonal, respectively. This is because plotting the ACS is even better tool for visualization of the resonances of all types than TSCS [6].

The plots in Fig. 4(a) correspond to the wave incidence along one of the cross arms. This means that the other two arms are illuminated in the broadside manner. The plasmon resonance of a single silver wire is known to sit at the wavelength of approximately 350 nm, slightly red-shifted from the value that provides $\mathrm{Re}\,\varepsilon(\lambda) = -1$. If the same wires are assembled into a linear grating, the main plasmon resonance could be still found at the same wavelength. From Fig. 4(a), one can also see that increasing the number of wires in the cross arm slightly inhibits the averaged value of ACS in the plasmon resonance. In contrast, under such illumination the principal grating-type resonances have the wavelengths slightly red-shifted from the period value, which has been taken, in computations, as p = 355 nm, i.e. just to the right from the plasmon resonance. Unlike plasmon, this resonance is getting sharper and more intensive if the number of wires increases.

If the plane wave illuminates the same cross of silver wires along its diagonal (Fig. 4(b)), the mentioned above features of the scattering and absorption are kept. The plasmon and the grating-type resonances are clearly identified by their different dynamics with respect to the growth of the number of wires. Here, the grating resonance is located near to the Rayleigh wavelength for the grazing regime of the +2-nd Floquet harmonic.

In Fig. 4(c), presented is the near-field amplitude pattern for a discrete cross made of 21 silver wires with radii 50 nm and period 426 nm at the grating resonance wavelength of 380 nm. One can see the field maxima and the standing waves at the illuminated side and the shadow zone at the opposite side of the cross.

IV. Conclusion

We have presented results of accurate calculations of scattering and absorption for three different periodically structured configurations made of silver nanowires, in the visible range. They demonstrate that corners and crosses of silver wires, if considered as a sensor assisted with combined plasmon-grating resonance, are less dependent on the direction of arrival of the incident illumination than a conventional linear chain of nanowires. This effect can find applications, for instance, in the design of more efficient plasmonic solar sells.

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