Grating Resonances on Periodic Arrays of Sub-Wavelength Wires and Strips: Historical Narrative and Possible Applications

(Invited Paper)

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Abstract: This paper reviews the history of discovery and the study of the nature of the high-quality natural modes existing on periodic arrays of sub-wavelength scatterers as specific periodically structured open resonators. Here, the arrays can be finite and infinite, and their elements can be dielectric and metallic. These grating modes (G-modes), like any other natural modes, are the "parents" of corresponding resonances in the electromagnetic-wave scattering and absorption. In the scattering cross-sections, they are usually observed as Fano-shape (double-extremum) resonances, while in the absorption they always display conventional Lorentzshape peaks. Thanks to high tunability, the G-resonances can potentially supplement or even replace the better known surfaceplasmon resonances in the design of nanosensors, nanoantennas, and nanosubstrates for surface-enhanced Raman scattering.

Noble-metal nanowires and nanostrips are known to display intensive surface-plasmon (SP) resonances in the visible range if illuminated with the H-polarized light (i.e. polarized orthogonally to the scatterer generatrix). The SP resonance wavelengths depend primarily on the shape of the scatterer cross-section. For instance, a sub-wavelength circular metal wire of dielectric permittivity ε_{met} located in the infinite host medium with $\varepsilon_h > 0$, has a single broad peak in the scattering and absorption cross-sections near the wavelength λ^{P} where $\operatorname{Re} \varepsilon_{met}(\lambda^{P}) = -\varepsilon_{h}$. The plane-wave scattering by such a wire can be studied analytically using the separation of variables. The resulting expressions can be further simplified using the small-argument asymptotics of cylindrical functions. This study shows that the wire possesses infinite number of closely spaced double-degenerate SP eigenmodes of azimuth orders $n \neq 1$, appearing as complex poles of the field as a function of the wavelength. However the corresponding resonance peaks overlap because the noble metals are lossy in the visible range, although the largest contribution comes from the dipole terms with $n = \pm 1$. Non-circular wire scattering analysis needs more elaborated techniques such as volume or boundary integral equations. They also reveal shape dependent SP-modes of different types and symmetries.

Thus the wavelengths of SP-resonances are specific for every metal and host medium that makes possible the "sensing" of the host medium refractive index by means of measuring of the SP wavelength. Still the Q-factors of SP-resonances are low, of the order of $\operatorname{Re} \varepsilon_{met} / \operatorname{Im} \varepsilon_{met} \approx 10$ in the visible range.

Although the pairs or small clusters of coupled metal wires or strips have been well documented, the optical properties of periodic ensembles of them, i.e. chains, arrays and gratings, remain less studied and their interpretation is still controversial. Here is a brief historical narrative of related publications.

The scattering of plane waves by free-standing infinite periodic gratings of *circular cylinders (wires)* made of metals and dielectrics has been extensively studied as a canonical scattering problem since the late 1890s [1-7].

It was in 1979 when K. Ohtaka and H. Numata reported, apparently for the first time, that the scattering of light by infinite one-period grating of thin dielectric cylinders showed narrow total-reflection resonances near specific wavelengths $\lambda_m^R = (d/m)(1 \pm \cos \beta), m = \pm 1, \pm 2,...$ depending on the period *d* and angle of incidence β [8]. However that effect did not attract any specific attention of research community. This is a good example of discovery that was done ahead of time and remained unclaimed for the next 25 years.

Although the G-resonances in the cases of both E- and Hpolarization can be noticed in the figures of papers published in the 1980s-2000s (for instance, Figs. 2 and 3 of [7], they became an object of specific investigation only in 2006 – see papers [9,10]. In these papers, the authors used the dipole approximation to show that total reflection resonances appeared just above the Rayleigh anomalies or "passing-off wavelengths," for a grating of thin dielectric wires. By that moment the manufacturing and measuring techniques have reached maturity, and soon the experimental verification of this effect was published in [11].

As known, the scattering resonances of various types are caused by the presence of the "parent" complex-valued poles of the field as a function of the wavelength while the Rayleigh anomalies are associated with the branch points and exist only for the infinite gratings. Therefore one can guess that the reason of overlooking the G-resonances in the most of studies before 2006 was their extreme proximity to the branch-point Rayleigh wavelengths λ_m^R , especially for thin-wire gratings.

Full-wave analysis of both wave-scattering and eignenvalue problems for the dielectric-wire gratings was presented in [12,13] and fully supported earlier findings of [8-10]. Effects of both G-resonances and SP-resonances on infinite gratings of silver wires (in the H-polarization case) have been studied numerically in [13,14]. In [14], new asymptotic expression for the complex-valued frequencies of G-modes has been derived; it has shown that if the wire radius or its dielectric contrast goes to zero then their natural frequencies go to the Rayleigh anomalies and the associated Q-factors rise to infinity. What is also new, in [12,13] it has been discovered that if the grating is made of quantum wires (i.e. can be pumped to display gain) then the G-modes demonstrate ultra-law thresholds of lasing that can be much lower than the threshold of the SP-mode.

It is interesting to check how these optical effects manifest themselves on finite gratings; such a study has been published in [21,22] for finite silver nanowire gratings. It has shown that the G-type resonances become visible in the reflectance and transmittance (see [21] for the definition of these quantities for finite gratings) provided that the number of wires is at least around N = 10. If it gets larger, the mode Q-factors tend to their limit values observed for infinite gratings. Important finding related to the case of high-quality G-resonance on a grating of many dozens or hundreds of wires tuned exactly to the wavelength of much lower-quality SP-resonance. In this situation, the presence of the G-mode induces a narrow band of optical transparency cutting through the much wider band of intensive reflection associated with the SP mode.

Flat gratings made of thin *noble-metal strips* have been always attractive in optics as easily manufactured components able to provide wavelength and polarization discrimination. The scattering by strip gratings had been initially studied (see [1,16-18]) assuming their infinite extension, zero thickness, perfect electric conductivity (PEC), and free-space location. Under these rude assumptions, the strip gratings show only the Rayleigh anomalies. In contrast, a gold-strip grating lying on a dielectric substrate displays both SP and G-resonances [19] provided that the substrate is sufficiently thick; and even a PEC-strip grating on a dielectric substrate has no SPresonances however has strong G-resonances, as found in [20].

The G-resonances on the free-standing *infinite* non-PEC strip gratings were found at first for thin dielectric strips in 1998 [21] and later for silver nanostrips [22] (see Figs. 1,2). In [22], it has been shown analytically that the wavelengths of G-modes tend to λ_m^R if the strip width or thickness gets smaller. Numerical study of both SP and G-resonances on finite gratings of silver strips has been published in [23].

It should be added that the G-resonances have been also studied theoretically and experimentally on the chains and various gratings of 3-D particles – see, for instance, [24-34].

The controversy around the G-resonances on various gratings of metal scatterers consists in the fact that, in the early studies, they were frequently mixed up with more conventional SP resonances. The failure to recognize their specific nature can be seen in the use of plasmon-related terminology such as "radiatively non-decaying plasmons," "supernarrow plasmon resonances," and "plasmon resonances based on diffraction coupling of localized plasmons." This started changing recently when the terms like "collective resonance" of [31-33] and "photonic resonance" of [34] appeared. Today it is known that the G-resonances exist in the scattering by the gratings of both metallic and dielectric elements and in the both of two principal polarizations. Hence it is clear they are caused solely by the periodicity and have nothing common with plasmons.

To highlight the inter-relation between the conventional SPresonances and G-resonances in the visible-light scattering by periodic noble-metal scatterers, we present some numerical data computed using the convergent algorithm, based on the analytical regularization [21], for an infinite grating of thin silver strips illuminated by a normally incident (i.e. along the *x*axis in Fig. 1(d)) H-polarized plane wave of the unit amplitude.



Fig. 1. Reflectance, transmittance, and absorbance as a function of the wavelength for the scattering of the H-polarized plane wave from the grating of silver nanostrips. The angle of incidence is $\varphi=0^0$, the strip width is 2w=150nm, the strip thickness is h=10nm, and the grating period is d=643nm.



Fig. 2. The near-field pattern on three periods for the scattering of the H-wave from the grating of thin silver nanostrips in the combined SP/G-resonance (λ =643.116nm). Other parameters are the same as for Fig. 1.



Fig. 3. The profile of the near field magnitude along the line y=0 for the scattering of the H-wave around combined SP/G-resonance at λ^{P} =643.116nm, λ =643.082nm, and λ =643.15nm. Other parameters are the same as for Fig. 1.

The dispersion of the complex dielectric permittivity of silver has been taken into account using the measured data for the both parts from the classical paper of Johnson and Christy.

The plots of reflectance, transmittance and absorbance as a function of the wavelength are presented in Figs. 1(a) and 1(b). They demonstrate two broad SP-resonances of enhanced reflection and absorption associated with the first and third-order standing-wave modes built on the short-range surface plasmon wave bouncing between the edges of each strip. Besides of them, one can see much sharper G-resonance at the wavelength slightly larger than the period; this resonance has the shape of reflectance minimum, i.e. leads to the optically induced transparency.

According to [22], in the normal-incidence case the normalized frequencies $\kappa = d / \lambda$ of the G-modes on material strip gratings are $\kappa_m^{GH} = m - m^3 (2\pi wh)^2 d^{-4} + O(|\varepsilon| m^4 h^4 d^{-4})$, where 2w and h are the strip width and thickness, respectively. If the incident wave length approaches the real part of the *m*-th natural G-mode wavelength, then the *m*-th Floquet harmonic amplitude a_m takes a large value not restricted by the power conservation law because it still exponentially decays in the

normal direction as $\operatorname{Re} \kappa_m < m$. In resonance, under the normal incidence, the optical field near the grating is dominated by the intensive standing wave built of two identical Floquet harmonics with numbers $\pm m$. For the plots in Fig. 1, m = 1 and $H \approx 2a_1 e^{ik\alpha_1|x|} \cos(k\beta_1 y) \approx Q_{G_1} \exp(-|x/d| Q_{G_1}^{-1}) \cos(2\pi y/d)$.

This is fully consistent with the near field patterns observed in Figs. 2 and 3. Note that in the G-resonance very large values of the near field stretch to the distance of some 50 periods on the both sides of the silver-strip grating and has the peak value of 95. This is ~25 times larger than in the SP-resonance whose near-field bright spots are small and stick to the strips [22].

In the case of finite silver-strip gratings, far field scattering patterns demonstrate intensive sidelobes in the plane of grating, explained by the mentioned Floquet modes excitation [23].

We have demonstrated that the grating or lattice resonances on the long periodic chains of finite number of wires or strips may have the Q-factors that are much higher than those usually associated with the plasmon resonances. These Q-factors grow up if the number of the grating periods gets larger. Therefore the grating resonances may serve as a superior alternative to localized surface plasmons for various applications in chemical and biological sensing and SERS. Their interplay depends on the angle of incidence, period of the grating, and the width and thickness of each strip. Choosing these parameters in optimal manner may help design periodic sensors, absorbers, and SERS substrates with improved characteristics.

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