

Chapter 4

Grating Resonances on Periodic Arrays of Sub-wavelength Wires and Strips: From Discoveries to Photonic Device Applications

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Abstract This chapter reviews the nature and the history of discovery of the high-quality natural modes existing on periodic arrays of many sub-wavelength scatterers as specific periodically structured open resonators. Although such modes can be found on various finite and infinite arrays made of metallic and dielectric elements, we concentrate our discussion around infinite arrays of silver wires and strips in the optical range. The grating modes (G-modes), like any other natural modes, are the “parents” of the corresponding resonances in the electromagnetic-wave scattering and absorption. Their wavelengths in either case are determined mainly by the period and the angle of incidence that has been a reason of their misinterpretation as Rayleigh anomalies. On the frequency scans of the reflectance or transmittance coefficients, G-mode resonances are usually observed as Fano-shape (double-extremum) spikes, while in the absorption they always display conventional Lorentz-shape peaks. If a grating is made of sub-wavelength size noble-metal elements, G-modes exist together with better known localized surface-plasmon modes (LSP-modes) whose wavelengths lay in the optical range. Thanks to high tunability and considerably higher Q-factors, the G-mode resonances can potentially supplement or even replace the LSP-mode resonances in the design of nanosensors, nano-antennas, and nanosubstrates for solar cells and surface-enhanced Raman scattering.

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4.1 Introduction

Noble-metal nanowires are known to display intensive localized surface-plasmon (LSP) resonances in the visible range if illuminated with the H-polarized light (i.e. polarized orthogonally to the scatterer axis). The LSP resonance wavelengths depend primarily on the shape of the scatterer cross-section. For instance, a thin circular metal wire of the relative dielectric permittivity ε_{met} located in an infinite host medium with $\varepsilon_h > 0$ has a single broad peak in the scattering and absorption cross-sections slightly above the wavelength value λ^P where $\text{Re } \varepsilon_{met}(\lambda^P) = -\varepsilon_h$. For a silver wire in free space, this yields $\lambda^P \approx 350$ nm [1]. The plane-wave scattering by such a wire can be studied analytically using the separation of variables and 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 LSP eigenmodes of the azimuth orders $n = 1, 2, \dots$, 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 $n = 1$. Non-circular wire scattering analysis needs more elaborated techniques such as volume or boundary integral equations. They also reveal shape dependent LSP-modes of different types and symmetries.

In scattering, LSP-resonances are the signatures of the underlying LSP-modes. If the shape of a metal wire is fixed, their wavelengths are specific for every host medium that makes possible the “sensing” of the medium refractive index by means of measuring the LSP wavelength [2]. The Q-factors of the LSP-resonances are low, of the order of $-\text{Re } \varepsilon_{met}(\lambda^P)/\text{Im } \varepsilon_{met}(\lambda^P) \approx 10$ in the visible range.

Although the optical properties of LSP modes of pairs (dimers) or small clusters of coupled metal wires or strips have been well documented [3], large periodic ensembles of them, i.e. chains, arrays and gratings, remain less studied and interpretation of the other, periodicity caused G-resonances is still controversial. Below we present a brief narrative of related publications and demonstrate the remarkable properties of these non-LSP resonances on nanogratings of circular wires and thin strips. For simplicity, the gratings are assumed to be suspended in free space.

4.2 Circular-Wire Gratings

The scattering of plane waves by free-standing *infinite* periodic gratings of *circular cylinders or wires* (see Fig. 4.1) made of metals and dielectrics has been extensively studied as a canonical scattering problem since the late 1890s [4–10]. Here, important research instrument was introduced by Rayleigh [5]: Floquet expansion of the field function in terms of spatial harmonics also called diffraction orders. Each Floquet harmonic is a homogeneous or inhomogeneous plane wave depending on the wavelength λ , period d and angle of incidence β .

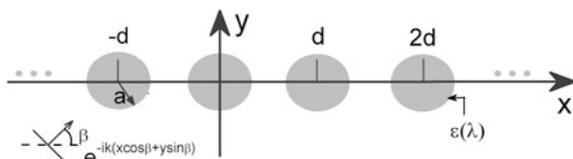


Fig. 4.1 Cross-sectional geometry of an infinite grating made of circular cylinders or wires

It was in 1979 when Ohtaka and Numata reported [11], apparently for the first time, that the scattering of light by an infinite one-period grating of thin dielectric circular cylinders showed unusually narrow total-reflection resonances. For the host medium with dielectric constant ε_h they appear near to (but not precisely at) the Rayleigh-Wood anomalies (RA) or “passing-off wavelengths,”

$$\lambda_{\pm m}^{RA} = (d\sqrt{\varepsilon_h}/m)(1 \mp \cos \beta), \quad m = 1, 2, \dots \quad (4.1)$$

These are the resonances on G-modes. However the found effect did not attract any specific attention of research community and remained unclaimed for the next 25 years. Thus, it is an example of discovery that was done ahead of its time.

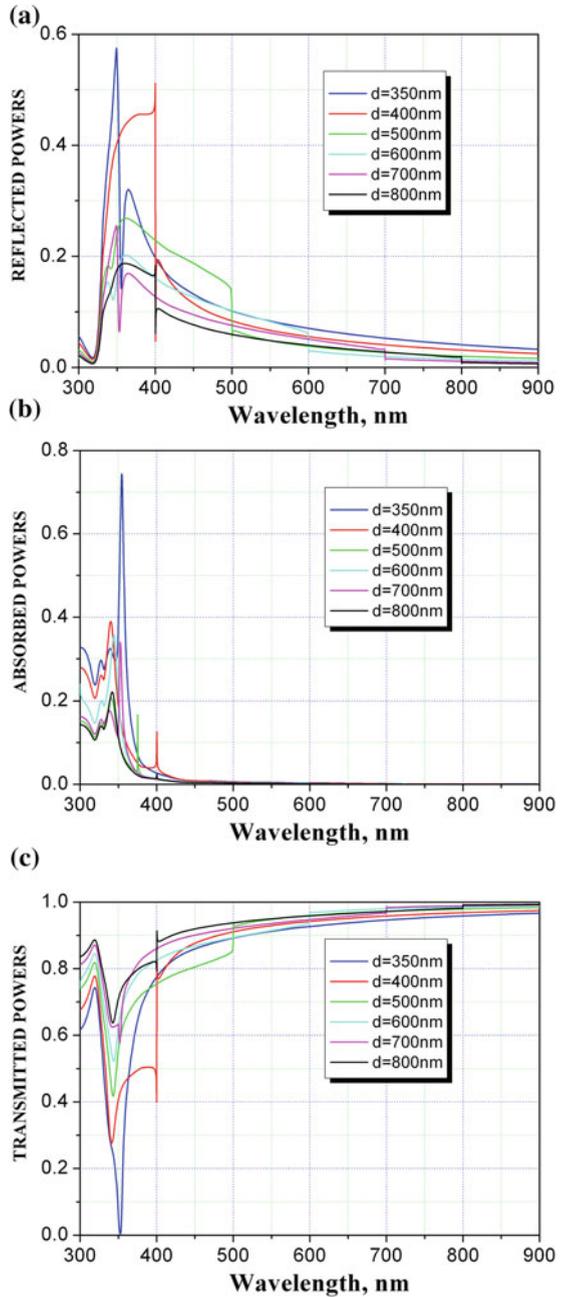
Although the G-resonances on dielectric-wire gratings in the cases of both E- and H-polarization can be noticed in some earlier papers (for instance, see Figs. 4.2 and 4.3 of [10]), they became an object of specific investigation only in 2006 [12–14]. In these papers, the authors used the dipole approximation to study the narrow total reflection resonances appearing on the extinction spectra just above the RA wavelengths. Experimental verification of this effect has been published in [15].

As already mentioned, 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. Unlike them, RAs are associated with the branch points and exist only for the infinite gratings. Therefore one can guess that the reason of the misinterpretation of the G-resonances in the studies related to infinite dielectric and metal wire gratings before 2006 was their extreme proximity to the RA branch-point wavelengths λ_m^{RA} , especially for the gratings made of thin wires.

Narrow resonances and high-Q eigenmodes need fine computational tools able to provide numerical results with many correct digits. Such a full-wave analysis of both wave-scattering and eigenvalue problems for the *dielectric-wire* gratings in free space was presented in [16, 17] using the meshless mode-expansion algorithm whose convergence is guaranteed. It refined earlier approximate results of [10–14].

Effects of both G- and LSP-resonances on infinite gratings of *silver* wires in free space (in the H-polarization case) have been studied numerically in [17, 18]. Here, the dielectric function ε_{met} was taken from [1]. Sample spectra of reflectance, transmittance and absorbance of silver-wire gratings are shown in Fig. 4.2.

Fig. 4.2 Spectra of reflectance (a), transmittance (b), and absorbance (c) of infinite circular silver wire gratings of different periods with wire radius $a = 48.85$ nm. H-polarization, normal incidence



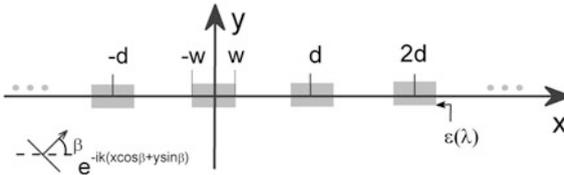


Fig. 4.3 Cross-sectional geometry of an infinite flat grating made of thin flat strips

As seen in Fig. 4.2, the LSP-resonance is present as a broad Lorentz peak near to 350 nm for all gratings. The G-modes usually display Fano-shape resonances in the reflectance and transmittance however simple Lorentz shape in absorbance. Important finding relates to the case of high-Q G-resonance on a grating of infinite number of wires with period tuned exactly to the wavelength of low-Q LSP-resonance. In this situation, the G-mode induces a narrow band of optical transparency cutting through the much wider band of intensive reflection associated with the LSP mode—see the curves for $d = 350$ and 700 nm.

In [18], new asymptotic expression for the complex-valued frequencies of G-modes was derived; it showed that if the wire radius or its dielectric contrast goes to zero then their wavelengths $\lambda_{\pm m}^G$ tend to the purely real RA wavelengths (4.1). Hence their Q-factors rise to infinity both for lossless and lossy wires.

In [16, 17] 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 that possess no RAs. Finite gratings of *many* thin wires remain relatively unclaimed area of research although early theoretical [6] and experimental papers [7, 19] noted unusual effects taking place near to the RA wavelengths. Accurate results of numerical study obtained by the convergent algorithm of [16, 17] have been published in [18, 20] for finite silver nanowire gratings where LSP and G-modes exist together. The resonances on G-modes become visible in the spectra of reflectance and transmittance (see [20] for the definition of these quantities for finite gratings) provided that the number of wires is at least $N = 10$. If it gets larger, the mode Q-factors tend to their limit values observed for infinite gratings.

4.3 Thin-Flat-Strip Gratings

Flat gratings made of thin *noble-metal strips* (see Fig. 4.3) have been always attractive in optics as easily manufactured components able to provide the wavelength and polarization discrimination. The scattering by strip gratings was initially studied assuming their infinite extension, zero thickness, perfect electric conductivity (PEC), and free-space location [4, 21–23].

Under these rude assumptions, the reflection and transmittance spectra of *infinite* gratings show only the RAs at wavelengths λ_m^{RA} . In contrast, a gold-strip grating lying on a dielectric substrate displays both LSP and G-resonances [24] provided that the substrate is sufficiently thick; and even a PEC-strip grating on a dielectric substrate has no LSP-resonances however has strong G-resonances [25].

The G-resonances on the free-standing *infinite* non-PEC strip gratings were found at first for thin dielectric strips in 1998 [26] although in the H-case narrow peaks of G-resonances were missed because of too coarse grid of computation points. This was clarified in the subsequent studies of impedance-strip [27] and silver-nanostrip [28] gratings. In [28], it has been shown analytically that the wavelengths of G-modes tend to λ_m^{RA} if the strip width or thickness gets smaller (see also (4.2) further in this section). Numerical study of both LSP and G-resonances on *finite* gratings of many silver strips has been published in [29–31].

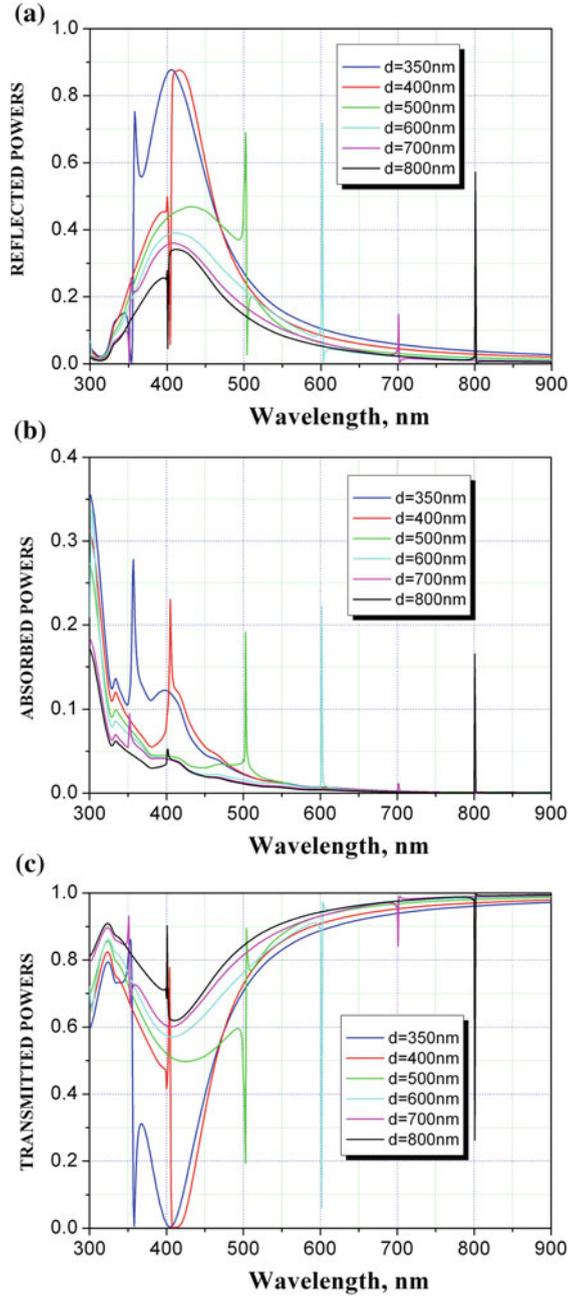
It should be added that G-resonances have been also studied theoretically and experimentally on chains and gratings of 3-D particles—see, for instance, [32–42].

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 LSP 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,” “subradiant lattice plasmons,” and “plasmon resonances based on diffraction coupling of localized plasmons.” This started changing recently when the terms like “collective resonance” of [39–41] and “photonic resonance” of [42] appeared. The fact that the G-modes and resonances exist in the scattering by the gratings of both metallic and dielectric elements and in the both of two principal polarizations makes it clear that they are caused solely by the periodicity and are not exotic plasmons.

To highlight the inter-relation between the conventional LSP-resonances 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 [28], for an *infinite* grating of thin silver strips illuminated by a normally incident H-polarized plane wave of the unit amplitude. The dispersion of the complex dielectric permittivity of silver has been taken into account using the measured data for the real and imaginary parts from [1].

The plots of reflectance, transmittance and absorbance as a function of the wavelength are presented in Fig. 4.4. The silver strip dimensions are taken as $50 \times 150 \text{ nm}^2$ that results in the same area of cross-section as for the circular wires corresponding to Fig. 4.2. They demonstrate one broad LSP-resonance of enhanced reflection and absorption at 410 nm, associated with the first-order standing-wave mode built on the short-range surface plasmon wave bouncing between the edges of each strip. Besides, one can see one or two much sharper G-resonances at the wavelengths slightly larger than the period and half-period of the grating; these resonances, if well separated from LSP-ones, display the Fano shapes (two closely spaced extremums). If the wavelength of one of them coincides with the LSP-mode, a narrow-band optically induced transparency is observed.

Fig. 4.4 Spectra of reflectance (a), transmittance (b), and absorbance (c) of infinite strip gratings of different periods with silver strip dimensions of $50 \times 150 \text{ nm}^2$, H-polarization, normal incidence

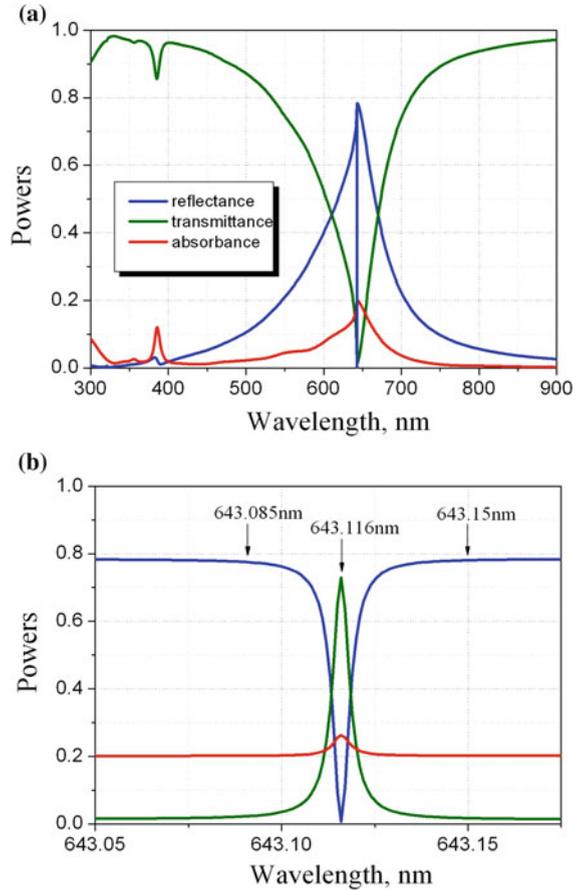


In Fig. 4.5, we demonstrate this effect in detail for the grating made of 10-nm thin silver strips. Such a reduced thickness is usual for today's nanotechnologies operating with electron-beam lithography and other techniques. Here one can see two broad LSP-resonances in the visible-light range around 640 and 380 nm, associated with the first and third-order LSP modes on each strip. Besides of them, one can also see an extremely sharp band of the optically induced transparency at the wavelength slightly larger than the period—see zoom in Fig. 4.5b. This is the effect of the G-mode resonance whose near-field patterns are shown in Figs. 4.6 and 4.7.

According to [28], in the normal-incidence case the normalized frequencies $\kappa = d/\lambda$ of the G-modes on a material strip grating with thickness $h/d \ll 1$ have the following asymptotic values:

$$\kappa_m^{GE,GH} = m - m^3(\chi_{E,H}2\pi wh)^2 d^{-4} + O(|\varepsilon|\chi_{E,H}^2 m^4 h^4 d^{-4}), \quad (4.2)$$

Fig. 4.5 Reflectance, transmittance, and absorbance spectra for the scattering of the H-polarized plane wave by infinite grating of silver nanostrips. The angle of incidence is $\beta = \pi/2$, the strip width is $2w = 150$ nm, the thickness is $h = 10$ nm, and the grating period is $d = 643$ nm



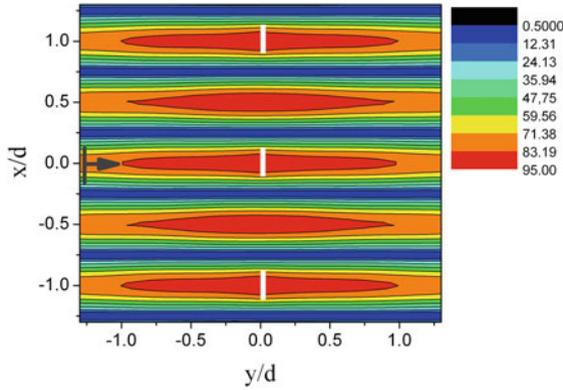
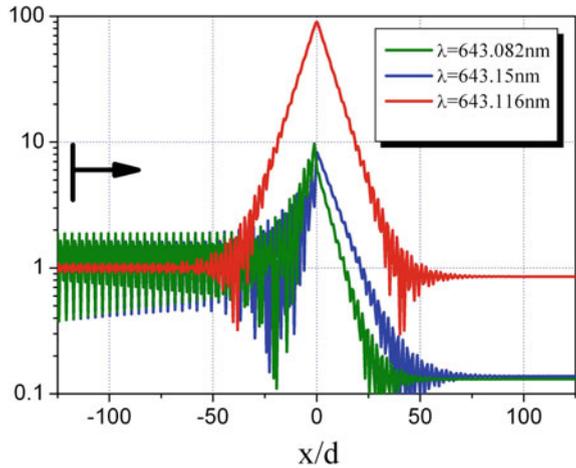


Fig. 4.6 The near-field pattern on three spatial periods for the scattering of the H-wave by infinite grating of thin silver nanostrips (shown using *white boxes*) in the combined LSP-G resonance ($\lambda = 643.116$ nm). Other parameters are the same as for Fig. 4.5

Fig. 4.7 The profile of the near field magnitude along the line $y = 0$ for the scattering of the H-wave around combined LSP-G resonance at $\lambda = 643.082, 643.116,$ and 643.15 nm. Other parameters are the same as for Fig. 4.5



where $\chi_E = \epsilon$ and $\chi_H = 1$. This means that, unlike LSP-mode, the G-mode quality factors $Q_m = -\text{Im} \kappa_m / 2\text{Im} \kappa_m$ tend to infinity if $h/d \rightarrow 0$ both for the lossy and lossless dielectric and metal materials in either polarization.

In the scattering problem, 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 proportional to the mode Q-factor. This value is not restricted by the power conservation law because $\text{Re} \kappa_m < m$ and hence the m th harmonic exponentially decays in the normal to the grating direction.

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. 4.5, $m = 1$ and hence

$$H \approx 2a_1 e^{ik\alpha_1|x|} \cos(k\beta_1 y) \approx Q_{G1} \exp(-|x/d|Q_{G1}^{-1}) \cos(2\pi y/d). \quad (3)$$

This is fully consistent with the near field patterns observed in Figs. 4.6 and 4.7. 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 the peak value is around 95. This is ~ 25 times larger than in the LSP-resonance whose near-field bright spots are small and stick to the strips [28].

In the case of *finite* silver-strip gratings, the G-mode near-field pattern is well visible along the grating except a few periods near the ends. Additionally, in-G-resonance far field scattering patterns demonstrate intensive sidelobes in the plane of grating, explained by the mentioned Floquet modes excitation [29, 30]. Note that Q-factors of G-modes on *finite* grating depend on the number of strips N .

4.4 Comparison Between Two Shapes and Two Polarizations

The LSP-mode resonances are always observed on the deep sub-wavelength metal scatterers with $\text{Re } \varepsilon_{met}(\lambda^P) < 0$. This is because the underlying physical phenomena have essentially static nature. Indeed, as it was shown in [43], the associated 2-D static problem of a non-magnetic cylinder in the uniform electric field possesses a set of discrete eigenvalues $\bar{\varepsilon}$ in terms of the dielectric constant. They depend on the shape of cylinder's cross-section and are negative real values. For a circular cylinder in free space, the single eigenvalue is $\bar{\varepsilon} = -1$, while for a rectangle it depends on the side lengths ratio. These eigenvalues have their projections to the H-polarized wave-scattering characteristics of the same 2-D metal scatterers whose dielectric permittivity is a function of the wavelength. The resonances on the LSP modes are found at the wavelengths near to those where $\text{Re } \varepsilon_{met}(\lambda) = \bar{\varepsilon}$.

Note that in the E-polarization case, duality of the magnetic and electric fields suggests that similar properties take place for the magnetic permeability function $\mu(\lambda)$. However for all non-magnetic objects, there are no eigenvalues of ε and hence no E-polarized LSP-modes and associated to them scattering resonances.

Keeping in mind manufacturing issues and applications, it is interesting to compare the characteristics of gratings made of comparable silver wires and silver strips. To verify the polarization selectivity of considered gratings, it is also necessary to compare the scattering and absorption by each type of gratings in two alternative polarization regimes. Such comparison is presented in Fig. 4.8.

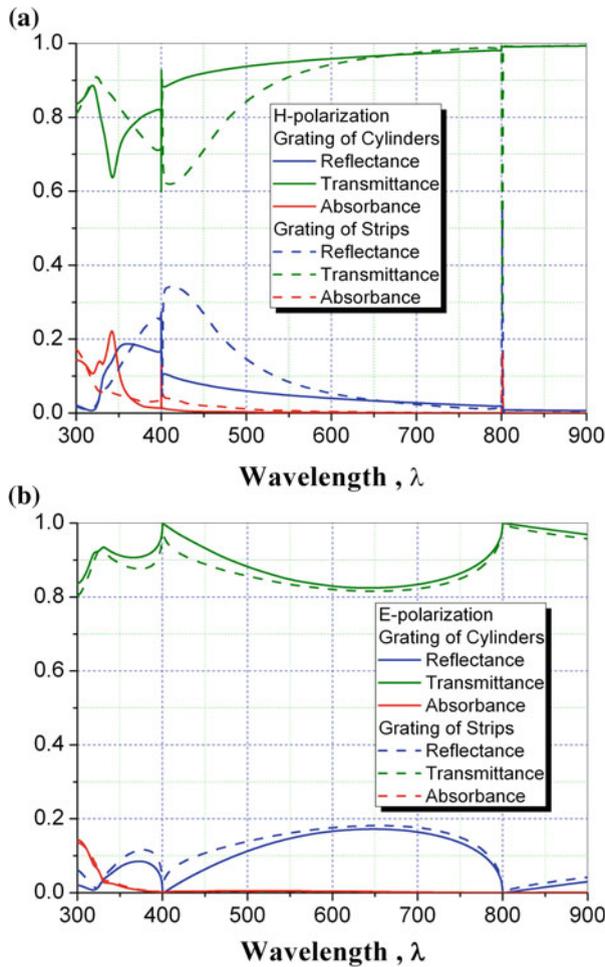


Fig. 4.8 Optical characteristics spectra of infinite silver gratings with period $d = 800$ nm illuminated by the H-polarized (a) and E-polarized (b) normally incident plane waves. The strip width is $2w = 150$ nm and the thickness is $h = 50$ nm, while the wire radius is $a = 48.85$ nm

Here the wire and strip have the same area of cross-section, and the period is fixed at $d = 800$ nm. As one can see, in the case of H-polarization (Fig. 4.8a) each grating displays a broad Lorentz-shape SP-resonance at the corresponding wavelength. Besides of that, each grating produces two super-narrow G-resonances at the wavelengths slightly red-shifted from the ± 1 -st and ± 2 -nd RAs in accordance to (4.2). Note that LSP-mode wavelengths are generally different however the G-mode ones agree well provided that the cross-sectional areas of elements are the same. The optical response to the G-modes varies from the universal Fano shape to the optically induced transparency after tuning to the LSP-mode wavelength.

In the case of E-polarization depicted in Fig. 4.8b, no resonances are visible. As mentioned above, no E-polarized LSP-mode poles exist on any metal grating. The G-mode poles, in contrast, exist for both dielectric and metal gratings in both polarizations—see [11–16, 26, 28]. The reason that they are not seen in Fig. 4.8b can be found on examining (4.2): the Q-factors of G-modes in the E-case are in $|\varepsilon|^2$ times lower than in the H-case that is a factor varying from 25 at 400 nm to 1100 at 800 nm. This “invisibility” of G-modes in the E-polarization scattering regime has apparently hindered correct identification of their nature because it had suggested that they might have something common to LSP modes, non-existing in this regime at all. Still if a metal nanograting is placed on a dielectric substrate, the G-resonances become visible in the E-polarization spectra as well [24, 25].

The only visible feature of the optical spectra of either grating in the E polarization is the transmittance maxima exactly at the RAs (4.1). The curves of equal-area gratings are very close to each other in the whole visible range. Note that the largest difference in the optical responses for two alternative polarizations takes place near to the H-polarization LSP and G-mode resonances for either grating.

4.5 Applications to Photonic Devices

One of the main applications of conventional localized LSP-resonances is the sensing of the changes of refractive index of the medium hosting a plasmonic scatterer [2]. This is performed by measuring the position of the peak scattering or extinction and considered as key enabling technology in biological and chemical nanosensors. Therefore it is not a surprise that remarkable properties of the recently verified G-mode resonances have immediately attracted attention of scientists and engineers designing the sensors based on metallic nanogratings. In this community, such devices are called (erroneously) “Rayleigh-anomaly sensors” apparently because of the nearness of the G-resonances to the RA wavelengths [44–47]. The paper [47] is remarkable for the expressed there confidence that these resonances and Rayleigh anomalies are different phenomena (although G-mode resonances are still interpreted as some specific plasmons). Such sensors were proposed in [46] where a concentric gold ring nanograting was placed on the facet of optical fiber. As the G-resonance wavelength is given, in the main term, just by the RA value of (4.1), one can expect very attractive linear dependence of the scattering peak on the refractive index. Then the sensitivity, in wavelengths per refractive-index-unit, equals to the grating period. This is true however only provided that the analyte material is infinitely thick, while in practice it is usually a liquid making a finite overlay. Hence the location of the G-mode peak strongly depends on the overlay thickness, so that thinner than the wavelength overlays seem impractical. Only for thicker overlays the refractive-index sensitivity approaches the ultimate bulk-index sensitivity value of such a sensor [47].

4.6 Conclusions

We have demonstrated and discussed the main features of the grating or lattice resonances on the periodic arrays of circular silver wires and strips. As it became clear rather recently, these resonances are caused by specific poles of the field function and the associated modes have much higher Q-factors than those of the LSP modes. Therefore the G-resonances may serve as a superior alternative to LSP ones for various applications in chemical and biological sensing, photovoltaics, and SERS. The interplay between two types of resonances depends on the angle of incidence and the grating period and to a lesser extent on the size of each wire or strip. Choosing these parameters in optimal manner may help design nanosensors, absorbers, and SERS substrates with improved features.

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