Electromagnetic surface states in structured perfect-conductor surfaces

F. J. García de Abajo\textsuperscript{1} and J. J. Sáenz\textsuperscript{2}
\textsuperscript{1}Centro Mixto CSIC-UPV/EHU and Donostia International Physics Center (DIPC), Apartado 1072, 20080 San Sebastian, Spain
\textsuperscript{2}Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Cantoblanco, 28049 Madrid, Spain
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Surface-bound modes in metamaterials forged by drilling periodic hole arrays in perfect-conductor surfaces are investigated by means of both analytical techniques and rigorous numerical solution of Maxwell’s equations. It is shown that these metamaterials cannot be described in general by local, frequency-dependent permittivities and permeabilities for small periods compared to the wavelength, except in certain limiting cases that are discussed in detail. New related metamaterials are shown to exhibit exciting optical properties that are elucidated in the light of our simple analytical approach.

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Structured metal surfaces offer a playground to yield remarkable optical phenomena ranging from extraordinary light transmission through subwavelength hole arrays \textsuperscript{1a} to innovative types of surface resonances \textsuperscript{2}. The relevant role of surface plasmons \textsuperscript{3} at visible and near-infrared frequencies was emphasized in early developments \textsuperscript{1b, 4}, while subsequent studies, following pioneering works in the field \textsuperscript{1c, 5}, demonstrated similar effects in plasmon-free good conductor films at microwave and THz frequencies \textsuperscript{6, 7}. Recently, these two regimes have been connected by the exciting prediction of Pendry et al. \textsuperscript{2} of surface resonances that mimic surface-plasmon behavior in perfect-conductor surfaces (PCS’s) textured with subwavelength holes, and by its subsequent experimental observation \textsuperscript{1d}.

Surface plasmons, originally predicted by Ritchie \textsuperscript{3}, have given birth to the rapidly growing field of plasmonics owing to their potential application in areas as diverse as biosensing \textsuperscript{10}, information processing via metal-surface circuits \textsuperscript{11}, or laser technology \textsuperscript{12}. Hence the importance of devising new ways to achieve surface-plasmon-like behavior in different frequency domains (e.g., using phonon-polaritons in the infrared \textsuperscript{13, 14}, or textured PCS’s at lower frequencies \textsuperscript{2, 15}).

In this Letter, we introduce a new approach to systematically study surface resonances in structured PCS’s. This allows us to provide further insight into recently proposed holey metamaterials \textsuperscript{2}, for which we find similar qualitative behavior and significant quantitative corrections in the surface mode dispersion relations. Furthermore, we show that this kind of materials cannot be represented in general by local, frequency-dependent optical constants [$\epsilon(\omega)$ and $\mu(\omega)$], except in some limiting cases. Finally, our results suggest a new systematics in the analysis of textured PCS’s that is applied to related metamaterial designs.

The material proposed by Pendry et al. \textsuperscript{2} consists of a planar PCS perforated by infinitely-long square holes of side $a$ arranged in a periodic square array of period $d \ll \lambda$ and filled with homogeneous material of permittivity $\epsilon_h$ and permeability $\mu_h$ ($\mu_h = 1$ will be used throughout this work), as sketched in the inset of Fig. \textsuperscript{1}. The assumption that the field inside the square-holes can be approximated by the lowest-frequency mode (i.e., the TE$_{1,0}$ mode \textsuperscript{16}), allows them to describe the bulk material by effective local optical constants $\epsilon_{\parallel}$ and $\mu_{\parallel}$ for fields parallel to the surface and $\epsilon_{\perp} = \mu_{\perp} = \infty$ for perpendicular fields (PMG model \textsuperscript{2}). In such an effective medium, the reflection coefficient for p-polarized incident light (external magnetic field parallel to the surface) is given by Fresnel’s equation

$$r_p = k_{\parallel} - k_{\parallel}/k_{\parallel} + k_{\parallel}/\epsilon_{\parallel}$$

where $k = \omega/c$ is the free-space light momentum, and $k_{\parallel}$ and $k_{\perp} = \sqrt{k^2 - k_{\parallel}^2}$ are the momentum components parallel and perpendicular to the surface, respectively. The surface resonances are signalled by the divergence of $r_p$ for incident evanescent waves ($k_{\parallel} > k$), leading to

$$k_{\perp}^2 = k_{\text{SB}}^2 = k^2 + \Gamma A^2 k_{\parallel}^4$$

with $A = a^2$ (the hole cross-section) and $\Gamma = 64\mu_h^2/\pi^6$ in the long-wavelength limit \textsuperscript{16}.

Fig. \textsuperscript{1} illustrates through a representative example a comparison between the PMG model \textsuperscript{2} (dashed curves) and a rigorous numerical solution of Maxwell’s equations obtained by expanding the electromagnetic field in terms of diffracted plane waves outside the surface and square-waveguide modes inside the holes. Our calculated results exhibit the same qualitative behavior as the PMG model in the long-wavelength limit (Fig. \textsuperscript{1}), although, as expected, the inclusion of diffraction orders outside the material introduces new structure in the high-frequency region and bends the dispersion relation at the boundary of the first Brillouin zone. Closer inspection into the long-wavelength region reveals a sizable correction in the
position of the resonance towards smaller values of \( k_\parallel \) (Fig. 1), quantified in a factor-of-3 larger decay length of the surface state into the vacuum. The physical origin of this discrepancy can be understood within the analytical approach that follows, corroborated by full numerical solution of Maxwell’s equations.

We consider a unit p-polarized plane wave incident along the \(xz\) plane (no surface modes are obtained for s polarization). The material will be contained in the \(z < 0\) region. In the absence of any surface structure, the total (incident plus reflected) field reads

\[
\begin{align*}
E^{\text{ext}}(r) &= \frac{2}{k} [i k_z \sin(k_z z) \hat{x} - k_\parallel \cos(k_z z) \hat{z}] e^{ik_z x} \\
H^{\text{ext}}(r) &= 2 \cos(k_z z) \hat{y} e^{ik_z x}.
\end{align*}
\]  
\tag{3}

Now, the small hole limit \((a \ll d, \lambda)\) allows representing each hole by effective dipoles. This was shown by Bethe \cite{bethe} for a single hole in a thin perfect-conductor screen, where the field scattered from the hole is proportional to that generated by an electric dipole perpendicular to the surface plus a parallel magnetic dipole, which are in turn proportional to the external perpendicular electric field and parallel magnetic field via the polarizabilities \(\alpha_E\) and \(\alpha_M\), respectively. Parallel electric dipoles and perpendicular magnetic dipoles are forbidden by the condition that the parallel electric field and the perpendicular magnetic field vanish at a PCS. A single hole in a semi-infinite PCS can be described in the same fashion. In the electrostatic limit, \(\alpha_E\) \((\alpha_M)\) can be calculated from the electrostatic (magnetostatic) solution for an external electric (magnetic) field, as shown in Fig. 2a (Fig. 2b), which involves only TM modes (TE modes) of the hole cavity.

The actual self-consistent field acting on each hole includes contributions from inter-hole dynamical interaction and symmetry considerations show that the magnetic and electric dipoles must be oriented as \(\mathbf{m} = m \hat{y}\) and \(\mathbf{p} = p \hat{z}\). Actually, \(\mathbf{m}\) and \(\mathbf{p}\) depend on hole positions \(\mathbf{R} = (x, y)\) just through phase factors \(e^{i k_z x}\). This permits writing the self-consistent relations

\[
p = \alpha_E [E_{z}^{\text{ext}} + G_{zz}^{\text{EE}} p + G_{yy}^{\text{EM}} m] \\
m = \alpha_M [H_{y}^{\text{ext}} + G_{yy}^{\text{EE}} m + G_{yz}^{\text{EM}} p],
\]  
\tag{4}

where \(G_{ij}^{\text{EE}}\) and \(G_{ij}^{\text{MM}}\) are lattice sums of the electric (E) and magnetic (M) dipole-dipole interactions, and \(i\) and \(j\) denote \(y\) and \(z\) Cartesian components. More precisely,

\[
\begin{align*}
G_{ij}^{\text{EE}} &= \sum_{\mathbf{R} \neq 0} e^{-ik_\parallel x} (k^2 - \delta_{ij}) e^{ik_\parallel R} \\
G_{yz}^{\text{EM}} &= -ik \sum_{\mathbf{R} \neq 0} e^{-ik_\parallel x} \delta_{xz} e^{ik_\parallel R}.
\end{align*}
\]  
\tag{5}

This inter-hole interaction is generally small for \(a \ll d\), except when a diffraction order goes grazing, in which case the above sums can diverge giving rise to phenomena related to Wood’s anomalies \cite{wood}. It is near these divergences that surface-bound modes can exist, subject to the condition

\[
(\alpha_E^{-1} - G_{zz}^{\text{EE}})(\alpha_M^{-1} - G_{yy}^{\text{EE}}) = (G_{yz}^{\text{EM}})^2,
\]  
\tag{6}

which is obtained from the vanishing of the secular determinant of Eqs. 3. In particular, near the light-line in the \(k_\parallel - \omega\) plane for \(k_\parallel > k\), one has

\[
\text{Re}\{G_{zz}^{\text{EE}}\} \approx \text{Re}\{G_{yy}^{\text{EE}}\} \approx \text{Re}\{G_{yz}^{\text{EM}}\} \approx \frac{2\pi k^2}{k_\parallel d^2} = S ,
\]  
\tag{7}

which comes from the divergent term of the parallel-momentum expansion of Eqs. 3 (see Fig. 3). Furthermore, upon inspection, one finds that \(\text{Im}\{G_{yz}^{\text{EM}}\} = 0\), and the remaining imaginary parts of all quantities in Eq. 3 cancel out exactly since \(\text{Im}\{G_{yy}\} = \text{Im}\{\alpha_E^{-1}\} = -2k^3/3\mu\), with \(\nu = E, M\). Combining these results, Eq. 3 can be approximated by Eq. 2 with

\[
\Gamma = \frac{4\pi^2}{A^3} \left( \frac{1}{\text{Re}\{\alpha_E^{-1}\}} + \frac{1}{\text{Re}\{\alpha_M^{-1}\}} \right)^2.
\]  
\tag{8}

Eq. 8 is exact in the \(a \ll d \ll \lambda\) limit, and it predicts the existence of surface-bound modes under the condition \(1/\text{Re}\{\alpha_E^{-1}\} + 1/\text{Re}\{\alpha_M^{-1}\} > 0\). Calculated values of \(\Gamma\) are offered in Fig. 2 for various systems. The position of the surface mode calculated from Eq. 8 (see Fig. 1) differs slightly from the exact numerical result, mainly due to neighboring-holes multipolar interaction for \(a = 0.8d\) (the holes occupy 64\% of the surface).

This description in terms of effective dipoles permits writing the specular reflection coefficient for p-polarized light as \(r_p = 1 + S(m - pk_\parallel /k)\). It is easy to see that this expression does not conform in general to the assumption of local optical constants implicit in the derivation of Eq. 1. In particular, for non-grazing incidence and \(\lambda \gg d\), the dipole-dipole interaction is neglected in Eqs. 3, so that using explicit expressions for the fields as provided by Eqs. 4, and noticing the \(r_p\) deviates only slightly from unity under these conditions, one finds

\[
\sqrt{k_\parallel/\epsilon_\parallel} \approx \frac{2\pi k}{d^2} (\alpha_M + \alpha_E k_\parallel/k)^2,
\]  
\tag{9}

which is independent of \(k_\parallel\) (i.e., of the angle of incidence) only if \(\alpha_E = 0\). Otherwise, the metamaterial is non-local, so that the optical constants of an equivalent homogeneous medium will depend on both frequency and momentum (spatial dispersion). It should be noted that the neglect of cavity modes other than the lowest-frequency one \((TE_1, 0)\) yields \(\alpha_E = 0\) (see Fig. 2), and therefore, it leads to an incomplete local-response description of the metamaterial \cite{metamaterial}.

From the point of view of external fields, the local-response picture will be still maintained if \(|\alpha_E| \ll |\alpha_M|\),
so that the second term in the right hand side of Eq. (9) can be overlooked. Such metamaterials can be achieved by filling the holes with media of very-high $\epsilon_h > 1$ or alternatively by using specific electrostatic resonances in the $-1 < \epsilon_h < 0$ range (piling up towards $\epsilon_h = -1$ as a manifestation of their filling-material surface-plasmon origin). This makes $\alpha_E$ negligible in the long-wavelength limit, as shown in Fig. 1.

Another possibility consists in filling dimples rather than holes using moderate values of $\epsilon_h > 1$ (e.g., $\epsilon_h = 10$ in Fig. 1) and $\lambda/d$. Indeed, the high-frequency propagating modes of infinitely-long holes become resonances of finite width (coupling to the external continuum) in holes of finite depth (dimples), which are blue shifted with respect to the noted propagating modes owing to reflection at the bottom and top ends of the hole (Fabry-Perot picture), as illustrated by comparing Fig. 3 and Fig. 1. For the choice of parameters of Fig. 3, there is a resonance in $\alpha_M$ near the lowest-frequency cavity mode ($\lambda = 7.2a$), where $\alpha_M$ is comparatively negligible. This dipole resonance provides a cut-off of surface-bound modes [2], as illustrated in Fig. 1. Higher-energy resonances of both TM and TE nature are also observed in the reflectivity, giving rise to a rich structure of surface-bound states (Fig. 1).

Similar behavior could be obtained by exploiting the mentioned single-hole electrostatic resonances. Optical phonons in alkali halides yield $\epsilon_h < 0$ [21] and can be combined with noble metals (near-perfect conductors) to implement these ideas in the THz domain. From Eqs. (3) and (5) and from the electric polarizability given in Fig. 5 the frequency dependence of $\epsilon_h(\omega)$ produces dispersion relations similar to Fig. 1 (not shown), including a cut-off due to the electrostatic resonances near $\epsilon_h = -1$.

The surface modes resemble surface plasmons not only in their limited penetration into the vacuum, but also in the interaction that they provide between additional surface features like holes of larger dimensions. Indeed, the scattered field produced by one of such features in the metamaterial decays away along the surface as $\exp(ik_R R)/\sqrt{R}$ at large distance $R$. This has the same form as the charge distribution accompanying a surface plasmon launched by a localized source [21], in contrast to the $\exp(ik_R R)$ far-field dependence of the interaction on unstructured PCS’s [22]. Furthermore, the far field of a small, localized additional surface feature can be assimilated to the field of an effective dipole placed at the surface of an equivalent homogeneous material with the same reflectivity as the holey metamaterial. Interestingly, in contrast to the dipoles that describe the underlying hole structure, the new effective dipole can have parallel electric and perpendicular magnetic components. This introduces another handle in the design of surface states by using the above holey metamaterials as the base fabric to build metamaterials drilled by larger holes, allowing us to speculate on surface modes in fractal structures that imitate Sierpinski’s carpet.

In conclusion, we have introduced a formalism to study textured perfect-conductor surfaces that allows us to obtain quasi-analytical long-wavelength exact dispersion relations for surface-bound modes. We have found that these metamaterials cannot be assimilated in general to equivalent effective homogeneous media described by local optical constants, except in some limiting cases (e.g., by filling the holes with high-index-of-refraction material). Finally, our results pave the way towards simple analysis of new metamaterial designs based upon the coexistence of different hole sizes and distributions that can realize the goal of achieving tailored surface dispersion relations.

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References:

[1] T. W. Ebbesen et al., Nature 391, 667 (1998).
[2] J. B. Pendry, L. Martin-Moreno, and F. J. García-Vidal, Science 305, 847 (2004).
[3] R. H. Ritchie, Phys. Rev. 106, 874 (1957).
[4] R. Gordon et al., Phys. Rev. Lett. 92, 037401 (2004).

FIG. 1: (a) Modulus of the specular reflection coefficient $|r_{sp}|$ of a perfect-conductor surface (PCS) perforated by infinitely-long square holes (see inset for parameters) as a function of wavelength $\lambda$ and momentum parallel to the surface $k_d$. The surface mode predicted in Ref. [2] is shown by a dashed curve. (b) Detail of the reflection coefficient $r_p$ along the AB segment of (a).

FIG. 2: (a) Electrostatic electric-field flow lines for a hole drilled in a semi-infinite perfect-conductor subject to an external field $E^{\text{ext}}$ perpendicular to the surface, giving rise to an electric dipole $p = \alpha_E E^{\text{ext}}$ as seen from afar. (b) Magneto-static magnetic-field flow lines for the same hole subject to an external parallel field $H^{\text{ext}}$ and leading to a magnetic dipole $m = \alpha_M H^{\text{ext}}$. (c) Summary of polarizabilities for square and circular holes in PCS’s, normalized using the hole area $A$. The circular hole in a perfect-conductor thin screen is analytical.

FIG. 3: (a) Dipole-dipole interaction sums for a square lattice of period $d$ [Eqs. (6) for $k_j \geq k$]. (b) Electric (solid curve) and magnetic (broken curve) polarizabilities of single holes filled with $\epsilon_h = 10$ material as a function of hole size. (c) Same as (b) for dimples.
FIG. 4: Inverse of the electrostatic polarizability of a single circular hole of area $A$ as a function of the dielectric constant $\epsilon_h$ of the filling material. The field strength distribution is shown in the insets for the two lowest-order resonances in the $-1 < \epsilon_h < 0$ range. The magnetostatic response is independent of $\epsilon_h$ ($A^{3/2}/\alpha_M \simeq 37.3$).

FIG. 5: Same as Fig. 1a for holes of finite depth $t = 1.5a$ filled with material of dielectric constant $\epsilon_h = 10$ (see inset).

[5] R. E. Collin and W. H. Eggimann, IRE Trans. Micr. Theory and Tech. 10, 110 (1961); C. C. Chen, IEEE Trans. Micr. Theory and Tech. 19, 475 (1971).
[6] R. C. McPhedran et al. (Springer-Verlag, Berlin, 1980).
[7] J. Gómez-Rivas et al., Phys. Rev. B 68, 201306(R) (2003).
[8] H. Cao and A. Nahata, Opt. Express 12, 1004 (2004).
[9] A. P. Hibbins, B. R. Evans, and J. R. Sambles, Science 308, 670 (2005).
[10] S. C. Schuster et al., Nature 365, 343 (1993).
[11] W. L. Barnes, A. Dereux, and T. W. Ebbesen, Nature 424, 824 (2003).
[12] R. Colombelli et al., Science 302, 1374 (2003).
[13] J.-J. Greffet et al., Nature 416, 61 (1999).
[14] R. Hillenbrand, T. Taubner, and F. Keilmann, Nature 418, 159 (2002).
[15] J. D. Jackson, Classical Electrodynamics (Wiley, New York, 1975).
[16] This value of $\Gamma$ is obtained assuming that $\omega$ is small compared to $\omega_{p1}$ in Eq. (12) of Ref. 2.
[17] H. A. Bethe, Phys. Rev. 66, 163 (1944).
[18] R. W. Wood, Phys. Rev. 48, 928 (1935).
[19] This exact, optical-theorem-like result is derived from flux conservation upon arbitrary external illumination for $k_0 > k$.
[20] Optical phonons can produce strong resonances in $\epsilon_h$, with very small $\text{Im}\{\epsilon_h\}$ near $\text{Re}\{\epsilon_h\} = -1$. See N. W. Ashcroft and N. D. Mermin, Solid State Physics (Holt, Rinehart, and Winston, New York, 1976).
[21] A. Kubo et al., Nano Lett. (2005).
[22] Flux conservation in 2D (3D) entails the $1/\sqrt{R} (1/R)$ dependence.
[23] Notice that Eq. 8 must be corrected by a factor of 4 in thin screens due to cooperative interaction between both sides of the film.
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