Plasmon-enhanced Bragg diffraction

Itai Epstein, Ido Dolev, Doron Bar-Lev, and Ady Arie[*]
Department of Physical Electronics, Fleischman Faculty of Engineering, Tel Aviv University, Tel Aviv 69978, Israel
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The diffraction from a single periodic metallic grating is shown to be significantly modified when a surface-plasmon polariton wave is excited at the metal-dielectric interface. In particular, vanishing diffraction orders in accordance with scalar diffraction theory, are generated in the presence of the surface wave. This modification is analytically explained, and a plasmonic Bragg law is formulated, which holds both in reflection and in transmission. Furthermore, when the metal layer is sufficiently thin, a dramatic increase in transmission is observed. If the grating is quasiperiodic, new diffraction orders, otherwise nonexisting, are created. We expect this general wave phenomenon to occur whenever a free-space wave is coupled to a surface wave through a periodic structure. Finally, new possibilities of plasmonic Bragg diffraction devices are presented.

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It has been almost 100 years since the formulation of one of the fundamental laws of physics, the well-known Bragg law.[1] Whereas, the original Bragg law was implemented for x-ray scattering from a periodic crystal lattice, it also had a tremendous impact in the field of optics by determining the scattering angles from a periodic structure. When the periodic structure is a metallic grating, some unique phenomena occur. Wood, in 1902, was the first to encounter anomalies in metallic diffraction gratings.[2] Lord Rayleigh referred to Wood's anomaly,[3] but it was Fano who pointed out the connection of these anomalies to surface waves.[4] Although Bragg law determines the possible diffraction angles from a periodic structure, the amplitude of each diffraction order is not derived. When the grating period is much larger than the wavelength, scalar diffraction theory approximation gives accurate results for the amplitude of each order.[5] When the grating period is much smaller than the wavelength, or at the wavelength scale, other methods, such as effective-medium approximation[6] and numerical simulations, can be used, and surface waves must be taken into account.

Surface-plasmon polaritons (SPPs) are surface waves that propagate at the interface between a dielectric and a metallic medium.[7] These surface waves, that exist only in TM polarization, are coupled to collective oscillations of electrons in the metal. Since the dispersion curve of SPPs lies to the right of the light line of the interface dielectric,[7] the momentum of the SPP is larger than that of the free-space electromagnetic (EM) wave. Therefore, an addition of momentum is required in order to couple (in or out) a free-space wave to SPPs. It is very common to excite SPPs using a metallic grating, whereby the grating provides the missing momentum.

Recently, we have demonstrated that the diffraction pattern of two different metallic gratings can be coupled by an SPP.[8] Using one grating to in-couple an SPP and the other to out-couple it, the SPP coupled the wave vectors of the two gratings. Furthermore, Yu *et al.*[9] have attracted great interest by demonstrating how SPPs can be used in order to modify the fundamental Snell law of reflection and refraction. In this paper, we experimentally demonstrate that Bragg diffraction from a single metallic grating is also significantly modified whenever an SPP wave is excited. Whereas, the Bragg law determines the possible orders, scalar diffraction theory determines which of these orders vanish due to the structure symmetries. However, when an SPP is excited, it modifies the diffraction pattern and leads to the generation of diffraction orders that, otherwise, are vanishing. Loewen and Popov[10] already explained the modification of existing diffraction orders by surface waves, but the generation of vanishing orders has not been considered until now.

The prediction of the possible angles, or orders, as formulated by Bragg,

$$\sin\theta_{\text{out}} = \frac{m\lambda}{\Lambda} - \sin\theta_{\text{in}}, \tag{1}$$

where θ_{in} and θ_{out} are the incident and diffracted angles, respectively, λ and Λ are the wavelength and grating period, respectively, and m is an integer, which represents the order number. For convenience, we rewrite Eq. (1) in terms of momentum as

$$k_{\text{out}} = mk_g - k_{\text{in}}, \tag{2}$$

where $k_{\text{in}} = k_0 \sin\theta_{\text{in}}$ and $k_{\text{out}} = k_0 \sin\theta_{\text{out}}$ are the projection of the wave vectors on the interface for the incident and diffracted waves, respectively, $k_0 = \frac{2\pi}{\lambda}$ is the free-space wave number, and $k_g = \frac{2\pi}{\Lambda}$ is the wave vector of the grating. The efficiency of the diffracted orders, which, owing to the symmetry of the grating's shape, determines the vanishing and existing orders out of the m orders of Eq. (1), yields that, for a binary grating with duty cycle (DC) $D = 50\%$, the existing orders are only the odd orders, whereas, the even orders vanish. In the same way, for the case of $D = 66\%$, the vanishing orders will be $m = \pm 3, \pm 6, \pm 9 \cdots$. However, if the grating period is on the order of the wavelength, in addition to scalar diffraction orders, the grating can also excite SPP waves. SPP coupling can occur through the grating, and the momentum conservation law in this case is as follows:

$$k_{\text{spp}} = k_{\text{in}} + nk_g, \tag{3}$$

where k_{spp} is the SPP wave number and n is an odd integer, as explained before.

Here, we consider the case of a grating that supports the momentum conservation of both Eqs. (2) and (3) simultaneously and, when illuminated by a free-space wave at a certain angle, both diffracts light directly and couples an SPP wave. This excited SPP wave at the interface also is diffracted by the grating into a free-space wave whose wave vector is as follows:

$$k_{\text{out}} = mk_g - k_{\text{spp}}, \tag{4}$$

where $k_{\text{out}} = k_0 \sin(-\theta_{\text{out}})$ under the conventional signs of diffraction theory. At this specific condition, Eq. (3) can be inserted into Eq. (4) to yield a modified relation between the wave vectors of the optical waves and the grating, i.e., a modified diffraction law,

$$k_{\text{out}} = (m-n)k_g - k_{\text{in}}. \tag{5}$$

For a grating with $D = 50\%$, Eq. (5) is similar to Eq. (2), but since m,n are odd, then $m-n$ is even, and the SPP wave is now being diffracted. This means that the vanishing even orders, in accordance with scalar diffraction theory, now are generated by the SPP. Another manifestation of the plasmonic law can be obtained by inserting Eq. (2) into Eq. (3) to yield the modified diffraction law,

$$k_{\text{out}} = (m+n)k_g - k_{\text{spp}}. \tag{6}$$

Again, $m+n$ is even, and Eq. (6) is similar to Eq. (2) with k_{in} being replaced by k_{spp}, denoting the SPP as the diffracted wave. Performing the same analysis for $D = 66\%$ by inserting the relevant m and n into Eq. (5) leads, in the same manner, to the generation of the otherwise vanishing $m = \pm3, \pm6, \pm9\cdots$ orders of the grating.

The expected "regular" and plasmonic Bragg diffraction patterns from two gratings illuminated with $\lambda = 1.064\ \mu$m at an angle of $\theta_{\text{in}} = 36.17^\circ$ with a period of $\Lambda = 2.5\ \mu$m and DCs of $D = 50\%$ and $D = 66\%$, which are addressed, hence, as D_1 and D_2, are presented in Figs. 1(a) and 1(b), respectively. The black, blue, and red arrows represent the incoming wave, the regular diffraction orders, and the generated SPP orders, respectively. It is important to emphasize that this is not a case where two independent beams illuminate the grating at two different angles, thereby producing two independent diffraction patterns, nor is it the case of one beam incident on a first grating to couple an SPP and then diffracted by a second grating where the gratings are independent (as demonstrated in Ref. 8). In our case, a single beam is incident on a single grating and produces the manipulation of Bragg's law as manifested in the diffraction pattern in a single process.

To verify this prediction, we have performed numerical simulations using rigorous-coupled-wave analysis (RCWA) as presented in Fig. 1(c). We simulated a silver binary phase grating ($\epsilon_m = -58.098\,98 + 0.6092i$) with a period of $\Lambda = 2.5\ \mu$m, D_1, and a height of $h = 70$ nm, on top of a 200-nm silver layer, surrounded by air and illuminated by a plane wave at a wavelength of $\lambda = 1.064\ \mu$m at two incident angles $\theta_{\text{in1}} = 34.15^\circ$ [red curve, Fig. 1(c)] where the SPP is almost nonexisting and, therefore, only the regular diffraction orders appear at angles θ_m: $\theta_{+1} = -7.8^\circ$, $\theta_{+3} = 45.72^\circ$, and $\theta_{\text{in2}} = 36.17^\circ$ [blue curve, Fig. 1(c)] in which the SPP coupling is maximal and, therefore, modifies the appearing diffraction orders to be θ_m: $\theta_{+1} = -9.47^\circ$, $\theta_{+2} = 15.15^\circ$, and $\theta_{+3} = 43.41^\circ$. It is clearly seen from Fig. 1(c), which is the Fourier decomposition of the cross section of the H_z field diffracted from the grating, that when an SPP is present, the otherwise vanishing $m = +2$ is generated and that it does not appear when the SPP is not present. Furthermore, it is also interesting

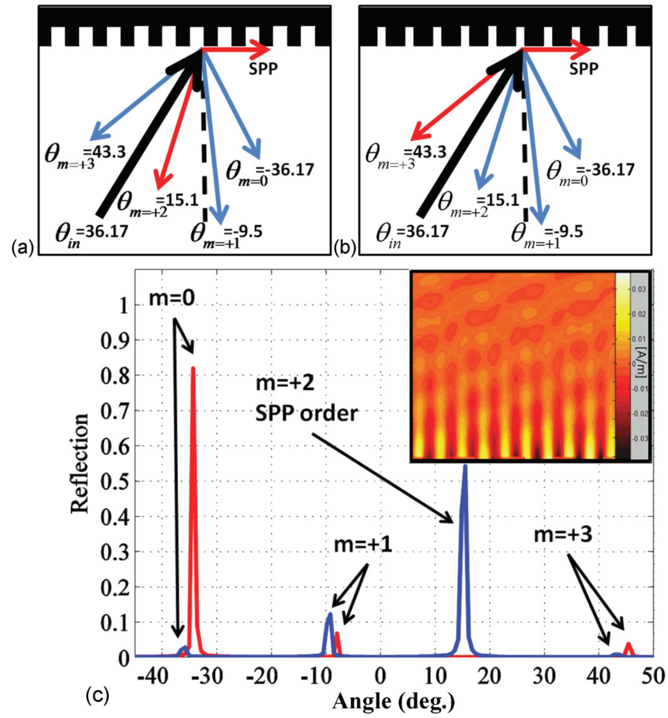

FIG. 1. (Color online) (a) and (b) Expected regular (blue arrows) and plasmonic (red arrows) diffraction orders from gratings D_1 and D_2, respectively. (c) Fourier decomposition of a cross section of the EM field diffracted from a simulated silver binary phase grating, illuminated by a plane wave at two incident angles: $\theta_{\text{in1}} = 34.15^\circ$ (red curve) where the SPP is almost nonexisting and $\theta_{\text{in2}} = 36.17^\circ$ (blue curve) where the SPP coupling is maximal. Inset: diffracted and SPP H_z fields (in $[\frac{A}{m}]$) from the RCWA simulation.

to observe the change in the zero order as it is almost eliminated by the transfer of energy to the SPP and its diffraction orders. This will be discussed in detail later on.

Sample preparation was performed by evaporating 200 nm of a silver film on a BK7 glass substrate, followed by standard electron-beam lithographic writing of the grating pattern on a polymethyl methacrylate (PMMA) mask. A 70-nm silver layer was evaporated above the PMMA, followed by a lift-off process to remove the undesired PMMA and metal. The result was two silver gratings with a period of $\Lambda = 2.5\ \mu$m and a height of $h = 70$ nm but with different DCs D_1 and D_2 and are presented in Fig. 2(a). To verify the effect of the different DCs, we illuminated the gratings with a green 532-nm laser, and the differences between the diffraction patterns of D_1 and D_2 can clearly be seen in Fig. 2(b). The efficiencies of orders $m = +2$ in D_1 and $m = +3$ in D_2, seen in Fig. 2(b), are negligible, and only faint diffraction is observed at these orders at the experimental wavelength, owing to the imperfection in the fabricated DCs.

The experimental setup, shown in Fig. 2(e), was composed of a 160-mW Nd:YAG cw laser ($\lambda = 1.064\ \mu$m), focused on the sample at a waist of $\sim$200 μm. The laser polarization was set by a half-wave plate, and a polarizer was set to TM polarization. The diffracted power was measured at a total range of 1.5° around the angle of SPP coupling at a step of $d\theta = 0.0215^\circ$. Figure 2(c) presents the diffraction patterns

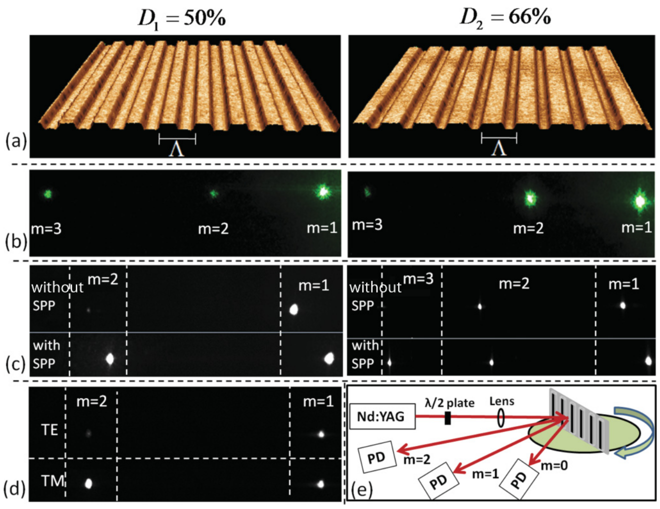

FIG. 2. (Color online) (a) A confocal microscope three-dimensional scan of D_1 and D_2. (b) The first three green laser diffraction orders of D_1 and D_2. (c) The difference between the diffraction patterns of D_1 and D_2 with and without the presence of an SPP. (d) The difference between the diffraction pattern of D_1 at TE and TM polarizations. (e) The experimental setup.

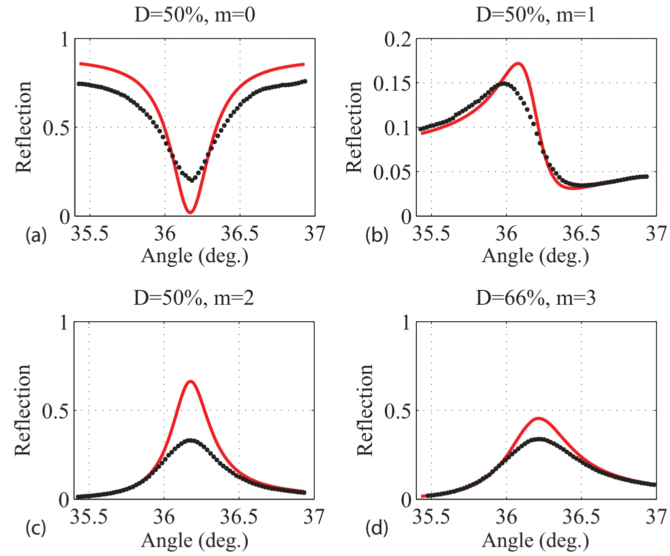

FIG. 3. (Color online) Measured (black marks) and RCWA simulations (red curves) of the angle-dependent reflection of (a) $m = 0$, (b) $m = +1$, and (c) $m = +2$ of D_1, respectively. (d) $m = +3$ of D_2.

from D_1 and D_2 at the angle of maximum coupled SPP power and at the angle where no SPP is excited. It is clearly seen that, when there is no SPP present, the $m = +2$ and $m = +3$ orders of D_1 and D_2, respectively, vanish, except for the negligible power related to the DC fabrication, whereas, at the angle of maximum SPP coupling, these orders are generated with significant power. Since SPPs can only exist in TM polarization, Fig. 2(d), which shows the diffraction pattern from D_1 at TM and TE polarizations, respectively, hereby verifies that this effect is indeed a plasmonic one.

Figure 3 presents the measured angle dependency (black marks) and RCWA simulation (red curves) for orders $m = 0$, $m = +1$, and $m = +2$ of D_1 and $m = +3$ of D_2. Figure 3(a) represents the $m = 0$ reflection curve, which exhibits a dip owing to the maximum coupling of the SPP at around 36.18°. Although the SPP coupling is maximized at this angle, the efficiencies of the vanishing orders $m = +2$ and $m = +3$ of D_1 and D_2, respectively, increase to a maximum as seen in Figs. 3(c) and 3(d). When further increasing the angle beyond that of a maximum SPP coupling, the process is restored back to regular diffraction. It is seen that the measured results are in good agreement with the RCWA simulations. The noticeable differences of the width and height between the measurements and the RCWA simulations are due to the imperfections, both in manufacturing of the gratings and in maintaining a pure TM polarization throughout the optical setup. Figure 3(b) shows the angular behavior of the existing $m = +1$ order of D_1 when an SPP is present. This behavior was already explained by Loewen and Popov,[10] and our results are in good agreement with their analysis.

By further investigating the single grating case, we found that this fundamental phenomenon can be expanded to virtually any metallic grating with two or more plasmonic orders, such as quasiperiodic gratings. One of these orders is used to couple in the SPP, which is then being diffracted by all the other orders. To validate this statement, we composed a grating of two pure sine waves with periods: $\Lambda_1 = 2.5$ and $\Lambda_2 = 1.7$ μm. Its modulation function is $h(x) = \frac{h_0}{4}[\sin(k_{g1} \times x) + \sin(k_{g2} \times x) + 2]$, where $h_0 = 70$ nm. Its reciprocal space and geometric form can be seen in Fig. 4(a) and the inset of Fig. 4(b), respectively.

Applying Eq. (5) to this grating, taking $m = n = 1$, and at an angle when an SPP wave is excited via k_{g1} yields, in the same manner as before, a new plasmonic-based diffraction order, having a wave vector,

$$k_{\text{out}} = k_{g1} - k_{g2} - k_{\text{in}}. \tag{7}$$

The expected regular diffraction orders from the grating, when illuminated at an angle of $\theta_{\text{in}1} = 35.64°$, are $\theta_{k_{g1}} = -9°$ and $\theta_{k_{g2}} = 2.5°$. This time, we simulated the diffraction from the grating using a commercial FDTD Lumerical software simulation. The grating was illuminated at angles $\theta_{\text{in}1} = 35.64°$ (red curve) where the SPP is maximal and $\theta_{\text{in}2} = 38.64°$ (blue curve) where the SPP is almost nonexisting. The Fourier decomposition of a cross section of the EM waves diffracted

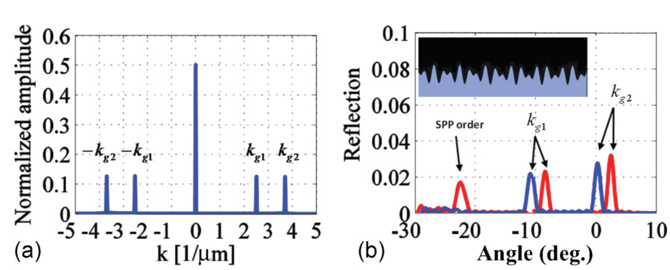

FIG. 4. (Color online) (a) Reciprocal space of the two sine gratings. (b) Fourier decomposition of a cross section of the EM waves diffracted from the structure. Inset: geometry of the two sine gratings.

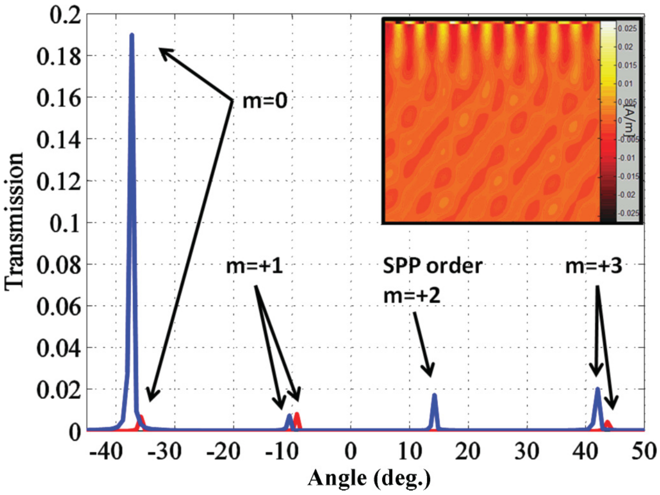

FIG. 5. (Color online) Fourier decomposition of the EM field transmitted through the grating with a thinner silver layer of 20 nm. Inset: the transmitted H_z field (in $[\frac{A}{m}]$).

from the structure for each illumination angle are presented in Fig. 4(b), and the generation of an additional plasmonic order at $\theta = -22.5^\circ$, corresponding to Eq. (7), is clearly seen. The zero orders are not presented as they are much higher than the others due to low SPP-coupling efficiency for this specific grating's parameters.

The modification of the diffraction spectrum also appears in transmission. We repeated the simulations of Fig. 1(c), but this time, the silver layer was reduced to a thickness of 20 nm instead of 200 nm, and the grating was surrounded from both above and below by air. The results are presented in Fig. 5, and it is clearly seen that the otherwise vanishing $m = +2$ order is again generated by the SPP. It is also clearly seen, similar to the phenomenon in reflection, that a dramatic change in the transmission of the zero order takes place. Although it is almost nonexisting without the presence of the SPP, it is enhanced dramatically when the SPP is present. The behavior of the zero diffraction order, both in reflection and in transmission, can be explained by destructive and constructive interferences between the free-space wave reflected/transmitted directly from the grating and the SPP diffracted wave from the grating.[11] At resonance, the system is nearly impedance matched, and the SPP coupling is maximal. At this point, the free-space wave that is directly reflected from the grating and the out-coupled SPP wave destructively interferes in reflection, thereby nearly eliminating the reflected signal and the zero order. The SPP wave is also out-coupled in transmission, thereby leading to dramatic enhancement in transmission. This enhanced transmission was previously reported in subwavelength hole metallic arrays,[12] but here, we show that it also occurs without any holes in the metal and requires only to have a metallic grating on top of the planar metal layer.

It is important to emphasize that the modification of the Bragg diffraction is a general wave phenomenon, not restricted to SPP waves only. We expect to see this effect for other types of free-space waves that are coupled using a grating for surface waves. An interesting example is the one for the case of acoustic waves. In recent years, it was shown that effects that were originally reported with plasmonic waves, such as extraordinary transmission through subwavelength holes,[12,13] have also been observed with surface acoustic waves.[14–16] Moreover, surface acoustic evanescent waves, analogous to surface plasmons, recently were experimentally observed.[17] Hence, we expect that the enhancement of the Bragg diffraction could also be observed with acoustic waves. It will also be interesting to extend this study to other types of surface waves, such as the ground radio wave, creeping waves, matter waves, etc.

Two conditions must be satisfied in order to observe the reported effect. First, the grating should couple a free-space wave into an SPP. This constraint is manifested in Eq. (3) and in terms of the structure's height-to-period ratio. The latter affects the SPP-coupling efficiency in several manners as described in the Supplemental Material,[18] which also shows that the phenomenon is observed for extremely large ranges of different grating heights (from 20 to 200 nm). Since the discussed phenomenon is based on the existence of the SPP wave, the power diffracted to the otherwise vanishing orders varies accordingly. Lastly, although we expect the phenomenon to suffer from plasmonic losses, it also is observed without losses (at longer wavelengths, for example).

The second constraint rises from the diffraction equation [Eq. (1)] since the sine function can take only values in the range of $[-1,1]$. This produces a constraint on regular diffraction in the term of the ratio among the wavelength, the structure's period, and the highest existing order: $\left|m\frac{\lambda}{\Lambda}\right| < 2$ and, therefore, limiting the highest existing mth diffraction order by the choice of the wavelength-to-period ratio. For example, consider a 50% duty-cycle grating, which has m odd regular orders and can diffract to even orders when an SPP is excited. For the 4th diffraction order to exist, we should satisfy $|m - n| = 4$ and, therefore, $|m| \geqslant 5$, which means that $\lambda < 0.4\Lambda$.

In conclusion, we have demonstrated that Bragg diffraction is significantly modified in the presence of SPP waves and that this modification can be formulated for a plasmonic Bragg law. SPPs can be used in order to manipulate diffraction patterns and to generate new, otherwise vanishing, orders both in reflection and in transmission, and the phenomenon can be extended to virtually any metallic grating having two or more plasmonic orders, such as quasiperiodic gratings. We expect that this phenomenon, being a general wave phenomenon, could be adopted for other waves. By optimizing the grating fabrication and choice of parameters, we can nearly eliminate the zeroth order in reflection and can enhance it in transmission, thereby enabling new plasmonic Bragg diffraction-based devices, such as a plasmonic polarization beam splitter in reflection, a plasmonic polarizer/attenuator in transmission, and a zero background signal (when the SPP is not excited) plasmonic-sensing device. Future work can be the expansion to two-dimensional plasmonics structures.

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*Corresponding author: ady@eng.tau.ac.il

[1]W. Bragg, Proc. Cambridge Philos. Soc. **17**, 43 (1912).
[2]R. W. Wood, Proc. Phys. Soc., London **18**, 269 (1902).
[3]Lord Rayleigh, Philos. Mag. **14**, 60 (1907).
[4]U. Fano, J. Opt. Soc. Am. **31**, 213 (1941).
[5]D. C. O'shea, T. J. Suleski, A. D. Kathman, and D. W. Prather, in *Diffractive Optics Design, Fabrication, and Test*, Tutorial Texts in Optical Engineering, Vol. TT62 (SPIE, Bellingham, WA, 2003).
[6]S. Rytov, Sov. Phys. JETP **2**, 466 (1956).
[7]S. Maier, *Plasmonics: Fundamentals and Applications* (Springer, New York, 2007).
[8]I. Dolev, I. Epstein, and A. Arie, Phys. Rev. Lett. **109**, 203903 (2012).
[9]N. Yu, P. Genevet, M. A. Kats, F. Aieta, J. P. Tetienne, F. Capasso, and Z. Gaburro, Science **334**, 333 (2011).
[10]E. Loewen and E. Popov, *Diffraction Gratings and Applications* (Dekker, New York, 1997).
[11]G. Diaz, N. García, and H. Raether, Surf. Sci. **146**, 1 (1984).
[12]T. W. Ebbesen, H. J. Lezec, H. F. Ghaemi, T. Thio, and P. A. Wolff, Nature (London) **391**, 667 (1998).
[13]T. Thio, K. M. Pellerin, R. A. Linke, H. J. Lezec, and T. W. Ebbesen, Opt. Lett. **26**, 24 (2001).
[14]M.-H. Lu, X.-K. Liu, L. Feng, J. Li, C.-P. Huang, Y.-F. Chen, Y.-Y. Zhu, S.-N. Zhu, and N.-B. Ming, Phys. Rev. Lett. **99**, 174301 (2007).
[15]H. Estrada, P. Candelas, A. Uris, F. Belmar, F. J. Garcia de Abajo, and F. Meseguer, Phys. Rev. Lett. **101**, 084302 (2008).
[16]J. Christensen, L. Martin-Moreno, and F. J. Garcia-Vidal, Phys. Rev. B **81**, 174104 (2010).
[17]Y. Zhou, M. H. Lu, L. Feng, X. Ni, Y. F. Chen, Y. Y. Zhu, S. N. Zhu, and N. B. Ming, Phys. Rev. Lett. **104**, 164301 (2010).
[18]See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.86.205122 for grating height-to-period ratio simulations.