

Self-referenced biosensor based on thin dielectric grating combined with thin metal film

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Abstract: Surface plasmon resonance biosensors based on grating coupling exhibiting two plasmons are less known because usually thick gratings and thick metal films are used. In this paper we show that when thin dielectric grating is used on top of thin metal film two surface plasmons are generated at the two boundaries of the metal film represented as two dips in the reflectivity or peaks in the absorption. One of the plasmons is sensitive to the analyte refractive index (sensitivity 580nm/RIU) while the other is sensitive to the refractive index of the substrate; hence it can be used as a reference. This self-reference makes the measurement more accurate and less sensitive to temperature fluctuations and optomechanical drifts. Field distribution calculations show that the plasmon excited at the metal-substrate interface is a long range plasmon with large penetration depth.

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OCIS codes: (050.1950) Diffraction gratings; (050.6624) Subwavelength structures; (280.4788) Optical sensing and sensors; (240.6680) Surface plasmons.

References and links

1. J. Homola, "Present and future of surface plasmon resonance biosensors," *Anal. Bioanal. Chem.* **377**(3), 528–539 (2003).
2. J. Homola, "Surface plasmon resonance sensors for detection of chemical and biological species," *Chem. Rev.* **108**(2), 462–493 (2008).
3. A. V. Kabashin, S. Patskovsky, and A. N. Grigorenko, "Phase and amplitude sensitivities in surface plasmon resonance bio and chemical sensing," *Opt. Express* **17**(23), 21191–21204 (2009).
4. K. M. Mayer and J. H. Hafner, "Localized surface plasmon resonance sensors," *Chem. Rev.* **111**(6), 3828–3857 (2011).
5. V. G. Kravets, F. Schedin, R. Jalil, L. Britnell, R. V. Gorbachev, D. Ansell, B. Thackray, K. S. Novoselov, A. K. Geim, A. V. Kabashin, and A. N. Grigorenko, "Singular phase nano-optics in plasmonic metamaterials for label-free single-molecule detection," *Nat. Mater.* **12**(4), 304–309 (2013).
6. D. Sinton, R. Gordon, and A. Brolo, "Nanohole arrays in metal films as optofluidic elements: progress and potential," *Microfluid. Nanofluid.* **4**(1-2), 107–116 (2008).
7. I. Abdulhalim, M. Auslender, and S. Hava, "Resonant and scatterometric gratings based nano-photonics structures for biosensing," *J. Nanophotonics* **1**(1), 011680 (2007).
8. O. Krasnykov, M. Auslender, and I. Abdulhalim, "Optimizing the guided mode resonance structure for optical sensing in water," *Phys. Express* **1**(3), 183–190 (2011).
9. S. F. Lin, C. M. Wang, T. J. Ding, Y. L. Tsai, T. H. Yang, W. Y. Chen, and J. Y. Chang, "Sensitive metal layer assisted guided mode resonance biosensor with a spectrum inversed response and strong asymmetric resonance field distribution," *Opt. Express* **20**(13), 14584–14595 (2012).
10. A. Mizutani, S. Urakawa, and H. Kikuta, "Highly sensitive refractive index sensor using a resonant grating waveguide on a metal substrate," *Appl. Opt.* **54**(13), 4161–4166 (2015).
11. D. V. Nesterenko, S. Hayashi, and Z. Sekkat, "Evanescent-field-coupled guided-mode sensor based on a waveguide grating," *Appl. Opt.* **54**(15), 4889–4894 (2015).
12. A. Shalabney and I. Abdulhalim, "Sensitivity enhancement methods for surface plasmon sensors," *Laser Photonics Rev.* **5**(4), 571–606 (2011).
13. V. Markel, "Coupled-dipole approach to scattering of light from a one-dimensional periodic dipole structure," *J. Mod. Opt.* **40**(11), 2281–2291 (1993).
14. S. Zou, N. Janel, and G. C. Schatz, "Silver nanoparticle array structures that produce remarkably narrow plasmon lineshapes," *J. Chem. Phys.* **120**(23), 10871–10875 (2004).

15. V. G. Kravets, F. Schedin, and A. N. Grigorenko, "Extremely narrow plasmon resonances based on diffraction coupling of localized plasmons in arrays of metallic nanoparticles," *Phys. Rev. Lett.* **101**(8), 087403 (2008).
16. B. Auguie and W. L. Barnes, "Collective resonances in gold nanoparticle arrays," *Phys. Rev. Lett.* **101**(14), 143902 (2008).
17. A. V. Kabashin, P. Evans, S. Pastkovsky, W. Hendren, G. A. Wurtz, R. Atkinson, R. Pollard, V. A. Podolskiy, and A. V. Zayats, "Plasmonic nanorod metamaterials for biosensing," *Nat. Mater.* **8**(11), 867–871 (2009).
18. A. Otto and W. Sohler, "Modification of the total reflection modes in a dielectric film by one metal boundary," *Opt. Commun.* **3**(4), 254–258 (1971).
19. J. Dostálek and J. Homola, "Surface plasmon resonance sensor based on an array of diffraction gratings for highly parallelized observation of biomolecular interactions," *Sens. Actuators B Chem.* **129**(1), 303–310 (2008).
20. A. Karabchevsky, O. Krasnykov, M. Auslender, B. Hadad, A. Goldner, and I. Abdulhalim, "Theoretical and experimental investigation of enhanced transmission through periodic metal nanoslits for sensing in water environment," *Plasmonics* **4**(4), 281–292 (2009).
21. A. Karabchevsky, O. Krasnykov, I. Abdulhalim, B. Hadad, A. Goldner, M. Auslender, and S. Hava, "Metal grating on a substrate nanostructure for sensor applications," *Phot. Nano. Fund. Appl.* **7**(4), 170–175 (2009).
22. A. Karabchevsky, M. Auslender, and I. Abdulhalim, "Dual-surface plasmon excitation with thin metallic nanoslits," *J. Nanophotonics* **5**(1), 051821 (2011).
23. K. Srivastava and I. Abdulhalim, "Self-referenced sensor utilizing extra-ordinary optical transmission from metal nanoslits array," *Opt. Lett.* **40**(10), 2425–2428 (2015).
24. C. J. Alleyne, A. G. Kirk, R. C. McPhedran, N. A. Nicorovici, and D. Maystre, "Enhanced SPR sensitivity using periodic metallic structures," *Opt. Express* **15**(13), 8163–8169 (2007).
25. M. Vala, J. Dostalek, and J. Homola, "Diffraction grating-coupled surface plasmon resonance based on spectroscopy of long-range and short-range surface plasmons," *Proc. SPIE* **6585**, 658522 (2007).
26. R. Magnusson, G. Svararsson, J. Yoon, M. Shokooh-Saremi, and H. Song, "Experimental observation of leaky modes and plasmons in a hybrid resonance element," *Appl. Phys. Lett.* **100**(9), 091106 (2012).
27. M. Auslender and S. Hava, "Scattering-matrix propagation algorithm in full-vectorial optics of multilayer grating structures," *Opt. Lett.* **21**(21), 1765–1767 (1996).
28. I. Abdulhalim, "Biosensing configurations using guided wave resonant structures," in *NATO Science for Peace and Security Series B: Physics and Biophysics, Optical Waveguide Sensing and Imaging*, eds. W. Bock, I. Gannot, and S. Tanev (Springer-Verlag, Dec. 2008), pp. 211–228.
29. A. Shalabney and I. Abdulhalim, "Electromagnetic fields distribution in multilayer thin film structures and the origin of sensitivity enhancement in surface plasmon resonance sensors," *Sens. Actuators A Phys.* **159**(1), 24–32 (2010).
30. Y. H. Kim, S. J. Park, S. W. Jeon, S. Ju, C. S. Park, W. T. Han, and B. H. Lee, "Thermo-optic coefficient measurement of liquids based on simultaneous temperature and refractive index sensing capability of a two-mode fiber interferometric probe," *Opt. Express* **20**(21), 23744–23754 (2012).
31. I. Abdulhalim, "Simplified optical scatterometry for periodic nanoarrays in the near-quasi-static limit," *Appl. Opt.* **46**(12), 2219–2228 (2007).
32. M. Rytov, "Electromagnetic properties of a finely stratified medium," *JETP Sov. Phys.* **2**, 466–475 (1956).

1. Introduction

Optical Biosensors are one of the most attractive and important optical devices, increasingly receiving huge interest in the last two decades [1], due to their importance in biology, chemistry [2,3], environment and industry. Among the extremely sensitive optical biosensors are the ones based on plasmonic nanostructures for example nanoholes, nanoslits, nanoparticles and more [4–6]. Resonant based structures are usually attractive because the resonance location (angle or wavelength) is usually easy to detect and in most cases its excitation is associated with evanescent wave. There are two important resonant phenomena used to design optical biosensors. The first phenomenon is the Guided Mode Resonance (GMR) [7,8], in which the structure consists of periodic dielectric grating coupled waveguide, illuminated with a specific wavelength and incidence angle at which the resonance condition is satisfied [7]. Sharp resonant peak exhibited in the reflectivity when the diffracted light matches the guided-mode condition causes interference with the zero-order beams, while on the other hand destructive interference occurs between the re-diffracted and the transmitted beams [7]. One of the unique features that make the GMR structures very useful is that the optical field is evanescent, and there is a sensing region where the resonance shifts due to variations in the refractive index within this evanescence region [7]. Other works proposed GMR on metal structures which consists of periodic dielectric grating (or periodic dielectric grating coupled waveguide) on the top of relatively thick metal film (>50nm) [9] or metal substrate [10]. In contrast to the conventional GMR structures, GMR on metal structures

showed dips in the reflectivity function because of the use of reflective/absorptive metal layer. In [11] a thin metal film was used but combined with thick dielectric grating under TE polarization. The second resonant phenomenon is the Surface Plasmon Resonance (SPR). There are two main types of Surface Plasmons (SPs), the first one is the extended or propagating surface plasmon resonance or (ESPR) which has been known for a longer time [12]. Extended SP is a longitudinal electromagnetic surface wave excited at and propagates along the interface between metal and dielectric and decays evanescently along the normal to the interface. The ESPR is excited with a specific wavelength and incidence angle when the resonance condition of momentum matching along the surface is satisfied causing a sharp reflection dip. Both in the GMR and ESPR, the resonance can be observed in two main modes, the angular mode (at fixed wavelength) and the spectral modes (at fixed angle), with the refractive index of the analyte changing due to pollution for example and causing shift of the resonance. The second type of SP waves is the localized surface plasmon resonance (LSPR) on the surface of nanoparticles and nanostructures that became very familiar during the last two decades. Several works showed theoretical [13,14] and experimental [15,16] collective coupling of localized plasmons in gold nanoparticle arrays. Due to their wide variety of applications such as in biosensing, nowadays a large number of theoretical and experimental research groups are active in the investigation of nanophotonic and nanoplasmonic metallic structures [17]. In order to excite LSPR in metallic structures, the dimensions of the structures should be less than half the wavelength of the exciting electromagnetic (EM) wave [12]. The present work concentrates on the ESPR.

There are a number of methods to excite ESPR, but the two main ones used in biosensing are using prism (Kretschmann-Raether [18]) and grating coupling [19]. In grating coupling there could be several possibilities: (i) the grating itself is metallic [20–25], (ii) the grating is dielectric on top of bulk metal [9,10,26], (iii) the grating is dielectric on top of thin metal film. In most of the works that used dielectric gratings (also GMR structures and SPR structures), the thickness of the grating was relatively thick, so in addition to the SPR excitation some GMR excitation was also observed [26]. In other cases the thickness of the Ag or Au metal film was relatively thick (>60nm) so that only one plasmon is excited [10].

In this work we demonstrate that using both thin dielectric grating (<200nm) and thin metal film (<50nm) two plasmons are excited, one on the top surface of the metal (adjacent to the interface with the analyte) and one on the bottom surface with the substrate. When the refractive index of the analyte is varied, the top plasmon location shifts according to the momentum matching condition while the bottom plasmon remains nearly fixed, so it can be used as a reference. Furthermore field distribution calculations show that the bottom plasmon is actually a long range plasmon. Hence a design is presented for self-referenced sensor in the near infrared region with a separation of ~80nm between the two plasmon wavelengths. As compared to the self-referenced sensor reported by our group recently (~160nm separation) based on enhanced optical transmission (EOT) [23] through nanoslits array, the present design has the advantage that a standard tunable laser can be used in the optical telecommunication window and the manufacturing of grating with features in the sub-micron regime is easier than features in the nanoscale regime (45nm).

2. Sensor design considerations and structure parameters optimization

Figure 1 shows a schematic diagram of the sensor based on dielectric grating on top of thin Ag film. The material of the dielectric grating lines is Si_3N_4 , the period of the dielectric grating is $\Lambda = 1000nm$ which is an important parameter that determines the resonance wavelengths location $\lambda_{res} = n_{eff}\Lambda$ where n_{eff} is the mode effective index. The chosen grating period gives resonance wavelengths in the near infrared region, the grating thickness is $h = 175nm$, the fill factor is defined by $f = W / \Lambda$ and equals to 0.55, the thickness of the metal film is $d = 40nm$ to allow the excitation of the two plasmons. The simulations showed

that this is the optimal thickness of the metal film and the contrast of the reference dip decreases and causes the measurement to be more difficult as the metal thickness increases. On the other hand by decreasing the metal film thickness, the reference dip becomes more sensitive to variations in the refractive index (RI) of the ambient of the analyte. The material of the substrate is SiO_2 chosen to give the reference dip as close as possible to the main dip. We present two possible designs, where in the first design the analyte is filling the spaces between the grating lines and on top of the grating. In the 2nd design in order to reduce the sensitivity of the reference dip to variations in the RI of the analyte, we filled the grating spaces with SiO_2 , on the cost of reducing slightly the contrast. The structure is designed to operate in the spectral mode at normal incidence under TM polarization for plasmons excitation.

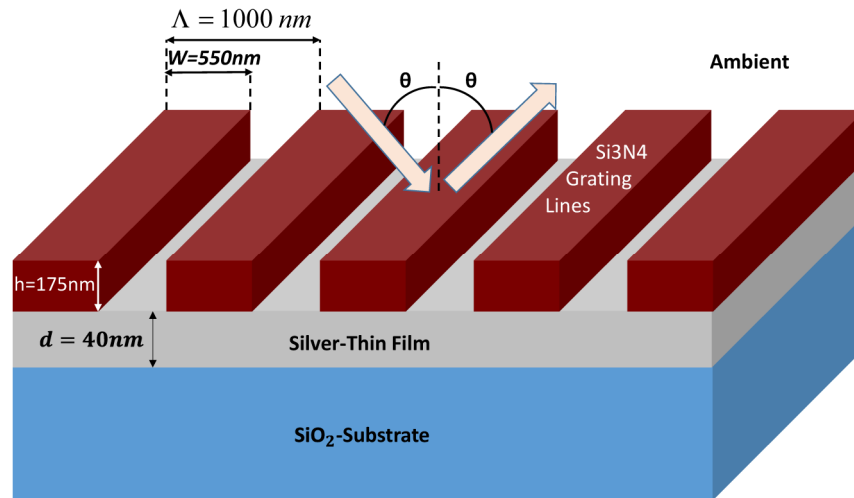


Fig. 1. Schematic diagram of the sensor based on dielectric grating on top of thin Ag film.

The main considerations during the sensor design and structure parameters selection were: (i) achieving reference dip with negligible sensitivity to the analyte RI, (ii) achieving high spectral sensitivity to the analyte RI (the non-reference dip), (iii) achieving high contrast, FWHM and figure of merit (FOM) for the two dips, (iv) achieving dips in the near infrared region, (v) achieving small spectral distance between the two dips so that tunable laser with short tuning range can be used.

3. Simulation methodologies

Rigorous electromagnetic simulations of gratings were used in this paper based on GSolver (see <http://www.gsolver.com/>) which is based on rigorous coupled-wave analysis (RCWA) method [27]. On the other hand in order to calculate the field distributions we used COMSOL software which is based on finite element analysis (FEA) method. We have verified that the reflection spectra calculated using GSolver and COMSOL are the same with very high accuracy. The refractive indices and the dielectric functions of the Ag (including the metal losses), SiO_2 and Si_3N_4 are taken from the database of GSOLVER. The data for the metal is based on experimental data but it fits very well the Drude model with damping. The incident light is a plane wave with TM polarization, the magnetic field amplitude at the input equals to one, the mesh size is extremely fine of 0.3nm (triangular mesh) and the boundary conditions are periodic.

4. Simulation results and discussions

4.1. Spectral response and field distribution calculation

4.1.1 Grating spaces filled with water

Figure 2(a) shows the spectral response of the self-referenced sensor for different refractive indices of the analyte in the case when the grating spaces filled with the analyte material (water in our case). One of the unique features of the sensor is that the reflection function has two dips, while only one of them is sensitive to the analyte refractive index variations. This means that the second one can be used as a reference because it remains nearly fixed due to variations in the RI of the analyte. This feature makes the measurement more accurate and less sensitive to temperature fluctuations and optomechanical misalignments, which improves the sensor stability and sensitivity. The proposed structure can be used as a sensor with a good spectral sensitivity of $580\text{nm} / \text{RIU}$. The second unique feature is the distance between the two dips which equals to 73.7nm , an important advantage because it allows the use of standard tunable laser used in the optical telecommunication window (usually operating in the range 1540nm-1620nm). The sensor showed good figure of merit, and good contrast of the dips, while the spectral sensitivity of the reference dip (the left one) to the analyte RI variations is $40\text{nm} / \text{RIU}$, which means that the right (non-reference) dip is sensitive to the analyte RI variations 14.5 times than the left one. This fact demonstrates that the left dip can be used as a reference, as shown in Fig. 2(a), when the RI of the analyte varies, the resonance wavelength red shifts according to the following equation: $\lambda_{\text{res}} = n_{\text{eff}} \Lambda$ that will be explained later. Figure 2(b) shows the total electric field distribution at normal incidence and $\lambda_{\text{res}} = 1536.2\text{nm}$, in the plane of incidence x-z. It is easy to see that most of the field is located in the analyte side and decaying in a direction that is normal to the surface (+z). Figure 2(c) shows the total magnetic field distribution at normal incidence and $\lambda_{\text{res}} = 1536.2\text{nm}$. It is important to note that in the COMSOL simulation we supplied magnetic field at the input with amplitude equals to one, so the ratio between the amplitude of the electric and the magnetic fields can be explained by the impedance of the media that the light is propagating in. At $\lambda_{\text{res}} = 1536.2\text{nm}$ an asymmetric plasmon is obtained because the major part of the field exists in one side of the metal. This plasmon is travelling at the surface of the top interface of the dielectric-metal and decaying in (+z) before getting absorbed in the metal film (large part of the field is located near the metal). The field distribution demonstrates that this resonance is sensitive to the grating lines, grating spaces and the analyte material because the field is mainly in these regions.

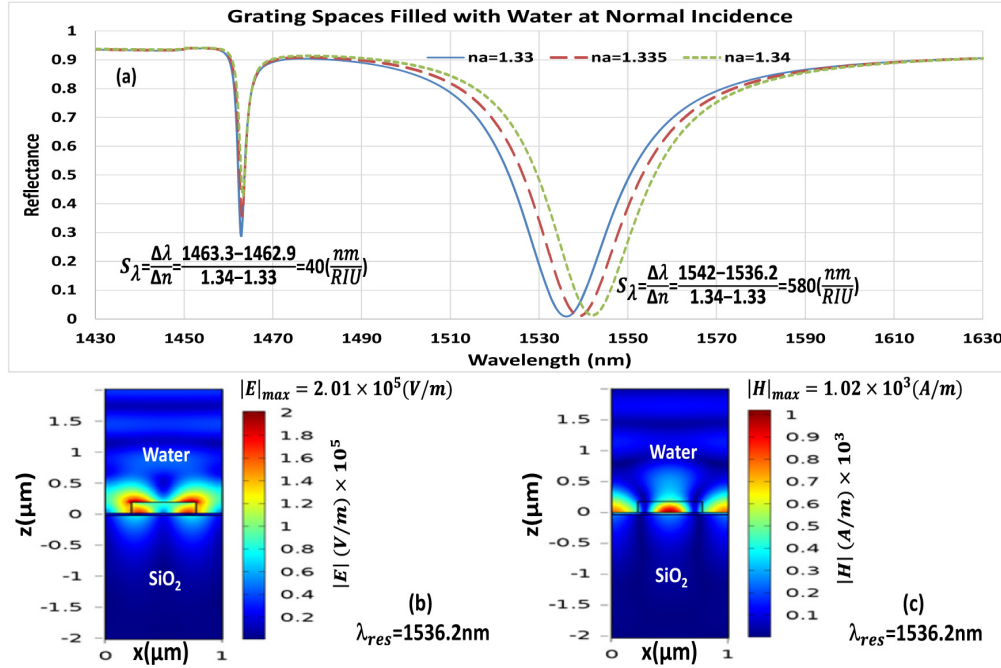


Fig. 2. (a) Spectral response (at normal incidence), for different refractive indices of the analyte. Field distribution at $\lambda_{res} = 1536.2\text{nm}$: (b) Total electric field, (c) Total magnetic field.

Figure 3(a) shows the spectral response of the self-referenced sensor for different refractive indices of the substrate in the case when the grating spaces are filled with the analyte material (water in our case). It can be observed in Fig. 3(a) that when the RI of the substrate increases, then the resonance wavelength of the reference dip red shifts. The spectral sensitivity of the reference dip (the left one) to the substrate RI variations is $950\text{nm} / \text{RIU}$ which is larger by a factor of around 1.64 than the spectral sensitivity of the right dip to the analyte RI variations. The reason for that is because the reference dip is a long range plasmon (LRSPR [25]) and it is penetrating for a depth of around $1.2\mu\text{m}$ inside the substrate. In other words the bottom plasmon has deeper evanescence field region relative to the evanescence field region of the top plasmon, so the interaction between this plasmon and the substrate material is more sufficient than the interaction of the top plasmon and the effective dielectric material at the top interface of the metal film. This fact demonstrates the correlation between the penetration depth which when increases also the propagation length increases and so also the sensitivity, through the increase of the overlap integral as was shown originally by our group [28,29]. Increasing the penetration depth has the advantage of improving the detectability of large bioentities such as bacteria; however it degrades the specificity of detecting small bioentities and molecules. This plasmon is travelling at the metal-dielectric interface for a longer distance relative to the top plasmon because most of the field is far from the metal surface and so absorbed less. We can estimate the propagation length according to

the following equation: $L_x \approx \frac{2\pi}{\Delta k_x}$ while L_x is the propagation length, k_x is the k-vector

component in x-direction which is defined by: $k_x = n_a k_0 \sin \theta$ where k_0 is the propagation constant in free space, n_a is the refractive index of the analyte and θ is the angle of the incident light. Now we can calculate Δk_x which is the FWHM in k_x -space, proportional to $\Delta \theta$ that defines the angular FWHM of the dip in the reflection function. We calculated $\Delta \theta$

from the angular mode and found that it is equals to 0.09 degrees. Using the previous relations and by substituting the parameters values, we can define and estimate the propagation length by the following equation: $L_x \approx \frac{\lambda}{n_a \cos \theta_{res} \Delta \theta} \approx 735.32 \mu m$ where λ is the wavelength of the

incident light and θ_{res} is the resonance angle in the angular mode. This propagation length is larger by about factor x5 the propagation length of extended SPR excited on silver-water interface in Kretschmann configuration; thus confirming that it is a LRSPR. Figure 3(b) shows the total electric field distribution at normal incidence and $\lambda_{res} = 1462.9 nm$, in contrast to the previous case, it is easy to see that in this case most of the field is located in the substrate side and decaying in the direction normal to the surface (-z). The field distribution in this case demonstrates that the reference dip is sensitive mainly to the substrate material, because the field exists nearly in the substrate side only. Similar to the right dip this one also asymmetric (in general LRSPR is an asymmetric mode). Figure 3(c) shows the total magnetic field distribution at normal incidence and $\lambda_{res} = 1462.9 nm$.

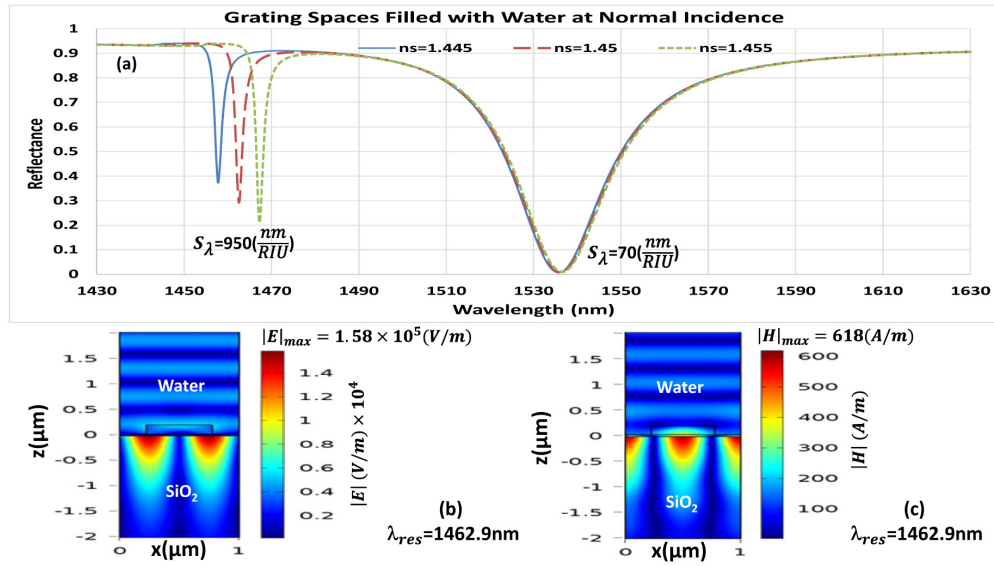


Fig. 3. (a) Spectral response (at normal incidence), for different refractive indices of the substrate. Field distribution at $\lambda_{res} = 1462.9 nm$: (b) Total electric field, (c) Total magnetic field.

The ESPR is excited with a specific wavelength and incidence angle when the resonance condition of momentum matching is satisfied causing a sharp resonant reflection dip. In order to calculate the absorption peaks that appropriate to the excitation wavelengths of the plasmons, we calculated the reflection and transmission functions and then the absorption is given by: $A = 1 - R - T$. Figure 4 shows the spectrum of the reflection, transmission and absorption functions in the case of grating spaces filled with water.

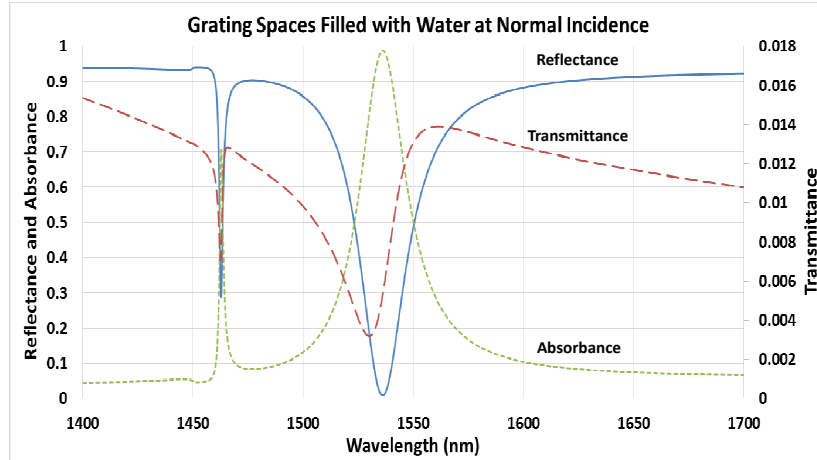


Fig. 4. Reflectance, transmittance and absorbance spectra at normal incidence, when grating spaces filled with water.

As it is observed in Fig. 4, according to the right side dip there is a small shift between the dip location of the reflection function, the dip location of the transmission function, and the peak of the absorption function. The reason for that is the strong dispersion and absorption of the metal that causes these shifts, which is a general phenomenon that can be observed when there is resonance combined with absorption. It is easy to see in Fig. 4 that the absorption function is asymmetric around the resonance, the reflection dip has a small red shift (relative to the absorption peak location), while the transmission dip has a small blue shift. It is important to note that at the resonance wavelength in the ideal case the reflection and the transmission functions should be equal to zero and the absorption function should be equal to one.

4.1.2 Grating spaces filled with SiO_2

In order to make the reference dip less sensitive to variations in the RI of the analyte, we filled the grating spaces with SiO_2 instead of the analyte material (water). Figure 5(a) shows the spectral response of the self-referenced sensor for different RIs of the analyte. The first noticeable result is that we get red shifts in the resonance wavelength of the right side dip, because, when the grating spaces filled with SiO_2 , the effective refractive index n_{eff} that affects the top palsmon becomes larger, and the resonance wavelength, which in general is given by $\lambda_{\text{res}} = n_{\text{eff}} \Lambda$ red shifts. More details as well as considerations to the homogenization method in order to calculate n_{eff} will be given later in the section dealing with dips location calculation. The spectral sensitivity of the reference dip (the left side one) to the analyte RI variations is $20\text{nm} / \text{RIU}$, which means that the reference dip became twice less sensitive than the reference dip in the case of the grating spaces filled with the analyte material. The spectral sensitivity of the right side dip to the analyte RI variations in this case is $490\text{nm} / \text{RIU}$ compared to the first case that was $580\text{nm} / \text{RIU}$. The contrast of the reference dip also decreases, but it is still high enough for measurement and similar to the first case, the sensor is showing good figure of merit. When the grating spaces were filled with water, the right side (non-reference) dip was sensitive to the analyte RI variations 14.5 times more than the left side one, when the grating spaces were filled with SiO_2 , the ratio between the two sensitivities to the RI variations of the analyte became 24.5, a fact which demonstrates that the left side dip became a more stable reference. In order to understand the importance of the reference dip for the measurement, we estimated the effect of the temperature on the dips

location. We calculated the reference dip shift due to 2°C drift in the room temperature, then the detection limit with the 2°C temperature drift was estimated in two cases. The first case is with the use of the reference dip, while the second is without using it. A tunable laser with 1pm resolution is assumed and the thermo-optic coefficient used of water at 1550nm according to [30] (worst case that causes a relatively large shift in the resonance). We found that by using the reference dip, the detection limit has improved by a factor of ~ 25 . Figure 5(b) shows the total electric field distribution at normal incidence and $\lambda_{\text{res}} = 1549.9\text{nm}$, similar to the first case, most of the field is located in the analyte side and decaying in a direction that is normal to surface ($+z$). Also one can see that in this case the penetration depth became smaller than the first case, as well as the amplitudes of the fields (in the substrate side) became smaller. The explanation to the reduction of these values together with the spectral sensitivities is that the analyte became more far from the top surface of the metal film where the top plasmon is excited. Figure 5(c) shows the total magnetic field distribution at normal incidence and $\lambda_{\text{res}} = 1549.9\text{nm}$.

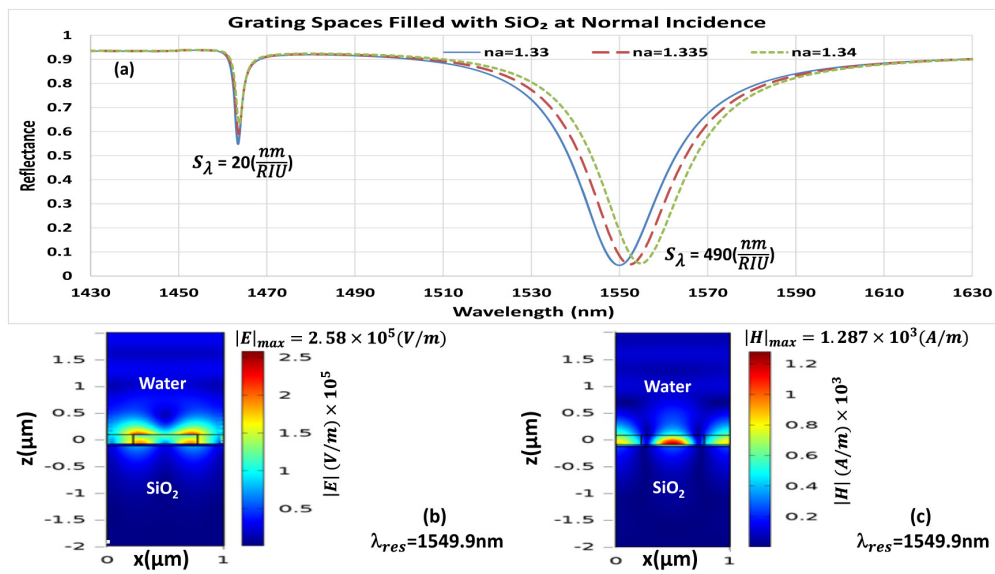


Fig. 5. (a) Spectral response (at normal incidence), for different refractive indices of the analyte. Field distribution at $\lambda_{\text{res}} = 1549.9\text{nm}$: (b) Total electric field, (c) Total magnetic field.

Figure 6(a) shows the spectral response of the self-referenced sensor for different RIs of the substrate for the case of the grating spaces filled with SiO_2 . The spectral sensitivity of the reference dip (the left side one) to the substrate RI variations is $970\text{nm} / \text{RIU}$ which is larger by a factor of around 1.98 than the spectral sensitivity of the right side dip to the analyte RI variations, Figs. 6(b) and 6(c) show the total electric and magnetic field distribution at normal incidence and $\lambda_{\text{res}} = 1463.5\text{nm}$ respectively. As mentioned before the reference dip is a long range plasmon and also when the grating spaces are filled with SiO_2 we paid in the spectral sensitivity of the right dip and its contrast. We can see the result of that in both cases in the field distribution calculations (Figs. 5(b) and 5(c), and Figs. 6(b) and 6(c)), and in particular it can be seen that the amplitudes of the fields (in the substrate side) and the penetration depths become smaller than the case of grating spaces filled with water. The reason for this is that the interaction region (the evanescent field region) becomes smaller.

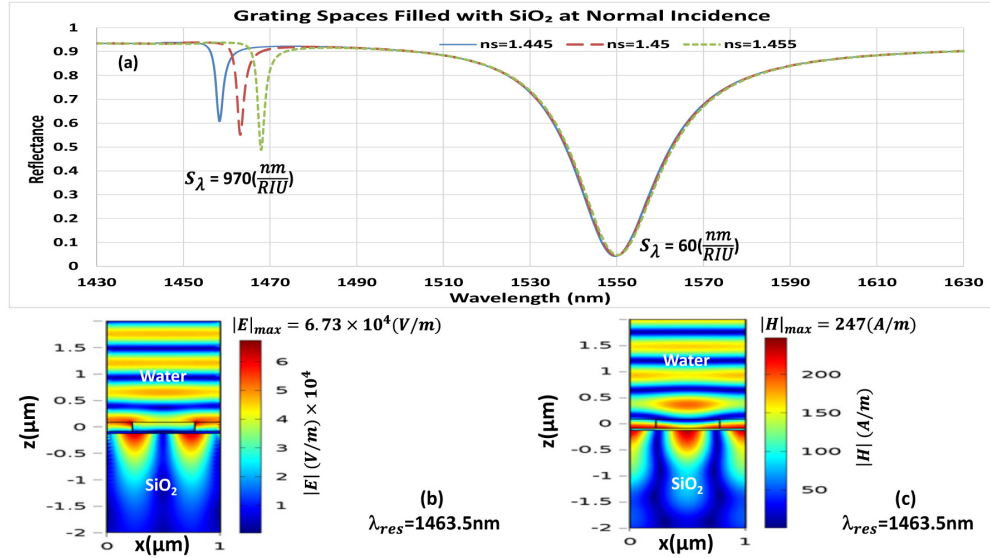


Fig. 6. (a) Spectral response (at normal incidence), for different refractive indices of the substrate. Field distribution at $\lambda_{res} = 1463.5nm$: (b) Total electric field, (c) Total magnetic field.

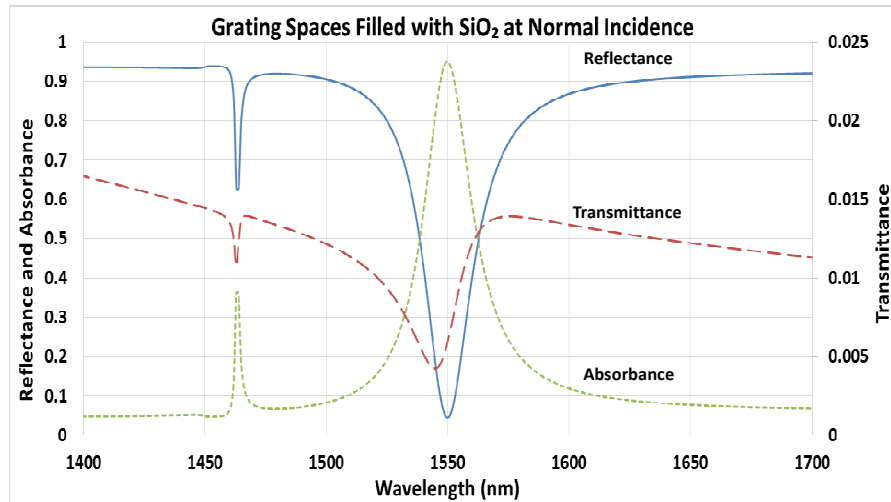


Fig. 7. Reflectance, transmittance and absorbance spectra at normal incidence, grating spaces filled with SiO_2 .

Figure 7 shows the spectra of the reflection, transmission and absorption functions in the case of the grating spaces filled with SiO_2 . Similar to Fig. 4, one can observe in Fig. 7 the shifts between the dip location of the reflection, transmission, and the absorption functions. In this case the absorption peaks are slightly smaller than in the case of the grating spaced filled with water. As mentioned before the reason is due to the reduction of the interaction region between the field and the analyte.

4.2. Metal film thickness effect

In order to investigate the effect of the metal film thickness on the reference dip, we simulated the spectral response of the sensor for different thicknesses of the metal thin film as well as

the total electric and the total magnetic field distribution calculations for grating spaces filled with SiO_2 . The results are shown in Figs. 8(a)-8(c).

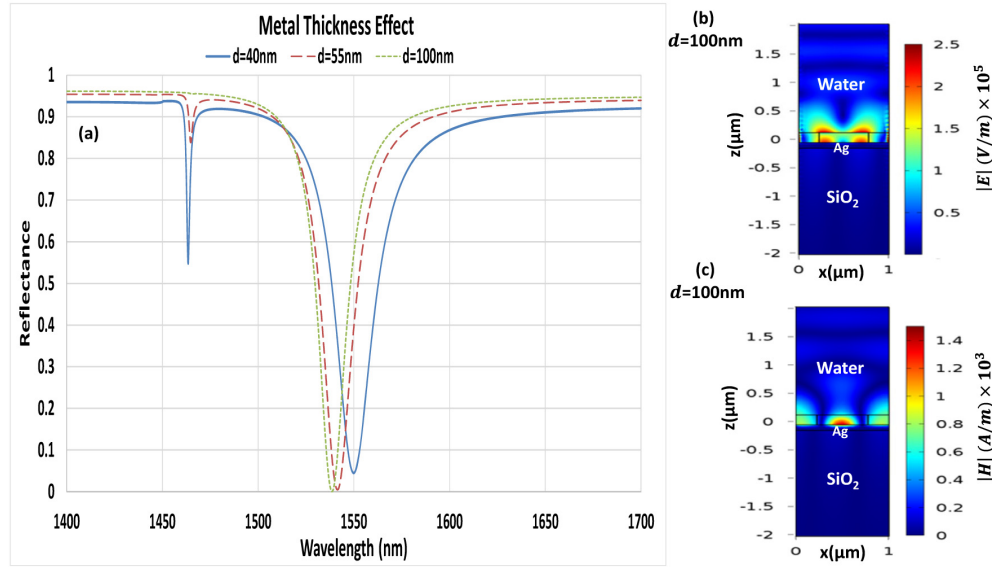


Fig. 8. (a) Spectral response (at normal incidence), for different thicknesses of the metal layer, grating spaces filled with SiO_2 . Field distribution at metal thickness $d = 100\text{nm}$: (b) Total electric field, (c) Total magnetic field.

As observed in Fig. 8(a), by increasing the thickness of the metal film the reference dip begins to disappear and at thickness around 100nm it is completely missing. The second observation is that the resonance wavelength of the right side dip is blue shifted. This is because the effective refractive index that affects the right side plasmon becomes smaller since when the metal layer thickness increases, the right side dip became less sensitive to the substrate material. The third observation is that now, there is more absorption by the thin metal film according to the right side dip. More details about the effective refractive index and its effect on the resonance wavelength will be presented in section 4.4. On the other hand by decreasing the metal film thickness, the reference dip became more sensitive to variations in the RI of the analyte. Our conclusion is that the optimal metal film thickness is 40nm in this case. Figure 8(a) is very important because it demonstrates the importance of the metal film thickness in order to allow physically the excitation of two plasmons, one on each interface.

4.3. At resonance vs. off resonance

In order to compare between resonance and off resonance cases we plotted the fields distribution for the total electric and the total magnetic fields in the two cases (at resonance $\lambda_{\text{res}} = 1549.9\text{nm}$ and off resonance at $\lambda_{\text{res}} = 1500\text{nm}$) when the grating spaces filled with SiO_2 . The results of the simulations are shown in Figs. 9(a) and 9(b) respectively. As it is shown in Fig. 9(b), in the off resonance case, we get travelling waves and the result of that is no evanescent wave, field strength is smaller and no possible sensing at this wavelength.

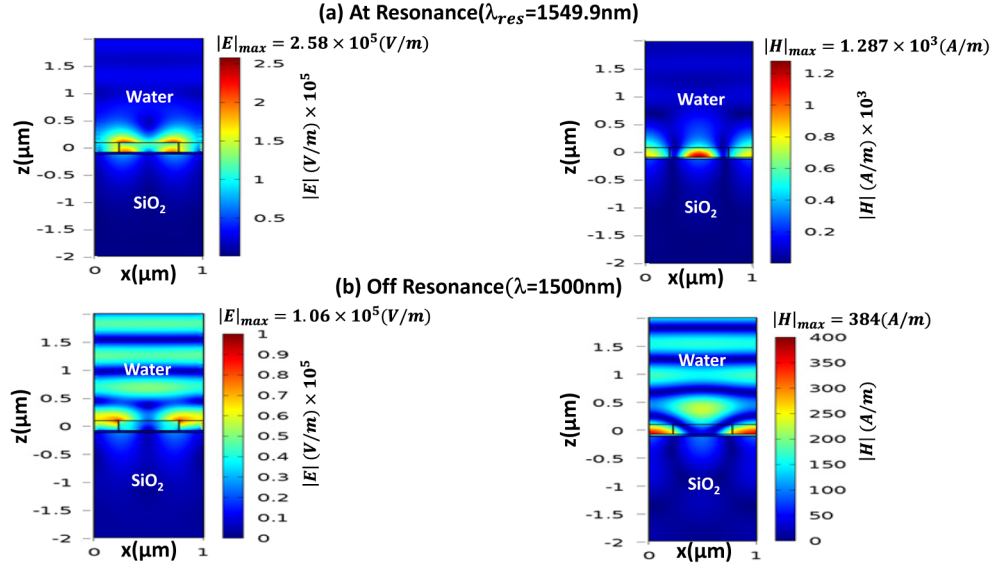


Fig. 9. Field distribution for the total electric and magnetic fields at normal incidence: (a) at resonance, $\lambda_{res} = 1549.9 \text{ nm}$, (b) off resonance, $\lambda_{res} = 1500 \text{ nm}$. Grating spaces filled with SiO_2 .

4.4. Analytical and numerical calculation of the resonance wavelengths location

In order to calculate the resonance wavelengths location, we start from the momentum matching equation along the interface: $k_{x_inc_light} + k_{Grating} = k_{SP}$:

$$k_0 n_a \sin \theta \pm m \frac{2\pi}{\Lambda} = k_0 \sqrt{\frac{\text{Re}(\epsilon_{metal}) \cdot n_{eff}^2}{\text{Re}(\epsilon_{metal}) + n_{eff}^2}} \quad (1)$$

At normal incidence and using $k_0 = 2\pi/\lambda$ from Eq. (1) we get:

$$\lambda_{res} = \pm \frac{\Lambda}{m} \sqrt{\frac{\text{Re}(\epsilon_{metal}) \cdot n_{eff}^2}{\text{Re}(\epsilon_{metal}) + n_{eff}^2}} \quad (2)$$

Where $k_{x_inc_light}$ is the k-vector of the incident light in x-direction, $k_{Grating}$ is the k-vector of the grating, k_{SP} is the k-vector of the surface plasmon, ϵ_{metal} is the complex dielectric constant of the metal, n_{eff} is the effective refractive index of the mode at the interface with the metal film, Λ is the grating period, m is the diffraction order and λ_{res} is the resonance wavelength. This means that we expect a linear relation between the resonance wavelength location and the grating period. At the bottom interface of the dielectric-metal, the resonance wavelength calculation is easy because, the plasmon at the bottom interface affected mainly by the material of the substrate. In this case the momentum matching equation is given by:

$$\lambda_{res_substrate} = \pm \frac{\Lambda}{m} \sqrt{\frac{\text{Re}(\epsilon_{metal}) \cdot n_{substrate}^2}{\text{Re}(\epsilon_{metal}) + n_{substrate}^2}} \quad (3)$$

Where $n_{\text{substrate}}$ is the refractive index of the substrate and $\lambda_{\text{res_substrate}}$ is the resonance wavelength of the bottom plasmon. At the top interface of the dielectric-metal, the case is more complicated for calculating the effective refractive index because we need to use the homogenization method valid at $\lambda/\Lambda \gg 1$ [31]. Based on a simple field averaging approach we can define the effective index as follows:

$$n_{\text{eff}}(x, z) = \frac{\int_0^h \int_0^\Lambda n_{g\text{-eff}}(x, z) E_{g\text{-eff}}(x, z) dx dz + \int_h^\infty \int_0^\Lambda n_a(x, z) E_a(x, z) dx dz}{\int_0^\infty \int_0^\Lambda E(x, z) dx dz} \quad (4)$$

Where $n_{g\text{-eff}}(x, z)$ and $E_{g\text{-eff}}(x, z)$ are the effective refractive index and the effective electric field in the grating region respectively, $n_a(x, z)$ and $E_a(x, z)$ are the refractive index and the electric field in the analyte region respectively. The electric field is a propagating wave in the x-direction and evanescent wave in the z-direction; therefore we write:

$$E(x, z) \propto \exp(-z/\delta) \exp(ik_x x) \quad (5)$$

Here δ is the penetration depth and k_x is the plasmon wave vector in the x direction. The effective refractive index of the grating ($n_{g\text{-eff}}$) is calculated according to the homogenization method up to the second order approximation of Rytov [32]. Within this approximation the subwavelength grating is replaced by a uniaxial layer with negative birefringence, which in the zero order approximation has the indices (for TE and TM polarization):

$$n_{TE0} = \sqrt{n_{SP}^2 (1-f) + n_g^2 f} \quad (6)$$

$$n_{TM0} = \frac{n_{SP} n_g}{\sqrt{n_{SP}^2 f + n_g^2 (1-f)}} \quad (7)$$

Then the second order approximation is given by:

$$n_{TE2} = \left\{ n_{TE0}^2 + \frac{1}{3} \left[\frac{\pi f (1-f) \Lambda}{\lambda} \right]^2 (n_g^2 - n_{SP}^2)^2 \right\}^{1/2} \quad (8)$$

$$n_{TM2} = \left\{ n_{TM0}^2 + \frac{1}{3} \left[\frac{\pi f (1-f) \Lambda}{\lambda} \right]^2 \left(\frac{1}{n_g^2} - \frac{1}{n_{SP}^2} \right)^2 n_{TM0}^6 n_{TE0}^2 \right\}^{1/2} \quad (9)$$

Here n_g is the refractive index of the grating lines and n_{SP} is the refractive index of the grating spaces, the effective refractive index in the grating region is given by: $n_{g\text{-eff}} = n_{TM2}$. Figures 10(a) and 10(b) show the analytical and numerical calculations of the resonance wavelengths for different grating periods at the top and bottom interface of the dielectric-metal film respectively.

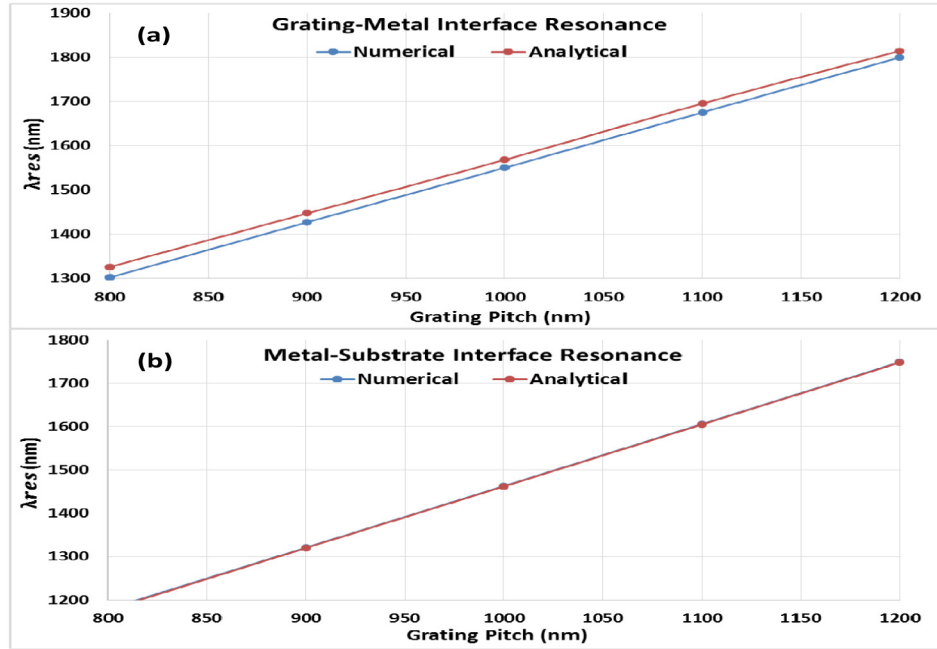


Fig. 10. Analytical and numerical calculations of the resonance wavelengths for different grating periods: (a) at the top interface of the dielectric-metal film, (b) at the bottom interface of the dielectric-metal film.

As it can be seen in Fig. 10(b), there is correlation between the analytic and numerical calculations of the resonance wavelengths at the bottom interface of the metal-dielectric film because the effective dielectric refractive index at this interface is simply the refractive index of the substrate $n_{substrate}$. Figure 10(a) shows that there is a small difference between the analytic and the numerical values at the top interface of the dielectric-metal film. The reason of this difference is because the homogenization method is not accurate enough, since the wavelength is not much larger than the grating period [31]. Figure 11 shows the magnetic field distribution for different grating periods. It is important to note that according to the momentum matching equation, when the effective refractive index becomes larger also the resonance wavelength becomes larger. The field intensities however do not change significantly as it can be seen in Fig. 11. The electric field carries the same information about the field distribution as the magnetic field.

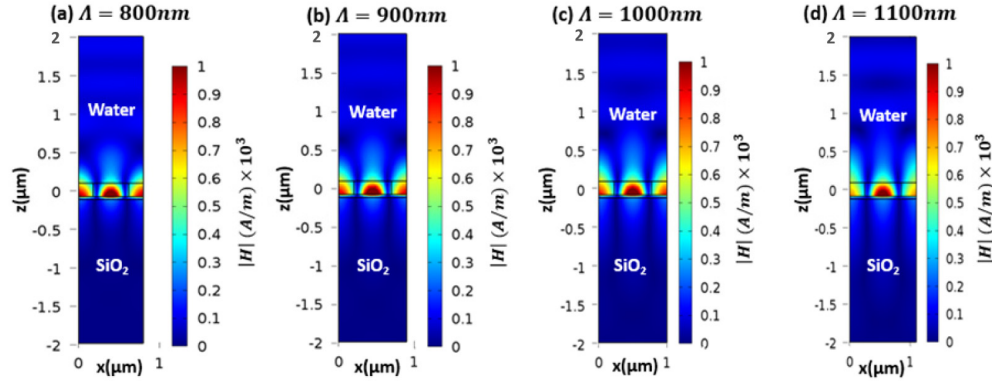


Fig. 11. Field distribution for the total magnetic field (at normal incidence) for different grating periods.

5. Analogy to the case of prism coupled low index dielectric layer and thin metal film

It is well known [12] that by inserting a low index dielectric layer (around 500nm thickness) between prism and thin metal film, it is possible to excite two plasmons at the two dielectric-metal interfaces. Our simulation showed that by decreasing the thickness of the grating to get very thin grating (few tens of nanometers), the right side dip disappears, and then we get only one plasmon at the bottom interface. However with the 175nm grating thickness we get two plasmons which we think have some analogy to the case of prism-dielectric-metal layer structure. Referring to the dielectric grating both as a grating coupler to help provide the momentum for plasmon excitation and as a dielectric layer, this structure can also support the excitation of two plasmons one at each dielectric-metal interface. The analyte in the prism coupling case is actually acting as the substrate in our case. The optimum thickness of the grating will depend on the wavelength, the grating, analyte and substrate refractive indices. One can use lower index grating but then its thickness is expected to be higher. The enhancement of the penetration depth and sensitivity of the LRSPP excited in both cases seem to be equivalent.

6. Conclusions and future works

The proposed structure of thin dielectric grating on top of thin metal film on substrate has two plasmonic modes in the reflection function, one of which can be used as a reference. The two resonances are excited at the two metal interfaces where one of them is a long range SPR. Field distribution simulations demonstrate the correlation between the existence of the fields in each case and the sensitivity of each resonance to the appropriate material RI. The advantages of the proposed structure are: (i) the use of thin dielectric grating with lateral features in the sub-microns scale and thin metal film instead of thin metallic nanoslits (40-50nm slits) array in the case of EOT which requires fine lithography process, (ii) the existence of reference dip, (iii) high spectral sensitivity, (iv) the distance between the two dips is smaller, (v) one of the plasmons is a long range with enhanced penetration depth so it can be used for large bioentities detection such as cells and bacteria. The long range SPR in the substrate medium can also be used for sensing with high sensitivity and large penetration depth, for example by replacing the analyte medium (ambient) with a medium of low refractive index such as MgF_2 while the substrate is replaced with a liquid medium of refractive index close to that of SiO_2 , which is possible for example as with blood medium. In the future we plan to study the angular behavior of such structure and to design sensors with new unique features observed from the angular response of the structure. We also planning to build such biosensor and confirm the observations experimentally in the near future.

Acknowledgments

This Research is conducted by NTU-HUJ-BGU Nanomaterials for Energy and Water Management Programme under the Campus for Research Excellence and Technological Enterprise (CREATE), that is supported by the National Research Foundation, Prime Minister's Office, Singapore.