



Dept of Physics, IIT Delhi

Course Code : PYD411

Academic Year : 2020 - 2021, Semester - II

Optimization of photonic crystal structure for sensors

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Adviser: Prof. Joby Joseph

Abstract: Demonstrating an analytical model for measuring change in Refractive index employing phase shift detection of GMR signal with acceptable sensitivity and presenting GMR tuning employing azimuthal Rotation.

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Signature of the adviser:

1 Introduction

Sensor Technology is one of the most widely used innovations, across fields ranging from Security tech to Bio technology and Scientific experimentation. With enormous Input taking capacities, New age sensors are dominating all kinds of usable devices which have extensive use in various fields associated with tasks ranging from enabling quality services to collecting hyper sensitive data for scientific purposes. On the abstract ground a sensor is a setup or device that is able to detect and report change in a certain predefined quantity. By looking through this lens, the area of exploration widens enormously. There are many types and classes of sensors which are already concretely established. for eg. Temperature, Proximity, Accelerometer, IR (Infrared Sensor), Pressure, Light, Ultrasonic Sensor, Smoke, Gas, Touch, Color, Humidity, Tilt, Flow and Level Sensors. On the frontier of sensing research are fields like Biosensing, Liquid sensing, Chemical sensing and Refractive index sensing. The crystal structure place a huge role in lot of these research, Guided mode resonance (GMR), based crystal structure are being widely researched upon in today's sensor technology. The amount of detailed sensitivity it provide with an acceptable range of wavelength to work with, it is a promising phenomenon. Currently there are variety of applications of this phenomenon available, including biosensing, which is the most widely used one (%cite%).

Guided Mode Resonance (GMR) is a resonance phenomenon where after diffraction from grating, particular diffracted order of the grating couples into waveguide and excites a guided mode in the waveguide. As the wave travels, it leaks out from the structure continuously. These leaky waves interfere with the 0^{th} order reflected wave. When certain phase matching conditions in these waves are met the interference produces a sharp peak in reflection spectrum. This GMR peak has a narrow line width, high efficiency and sensitivity towards change in surrounding refractive index (RI) due to which it is widely applied for bio-sensing and other sensing techonologies. the phase of GMR signal varies rapidly around the resonance peak, Due to this sensing based on phase detection have more potential than wavelength or angle-resolved in terms of limit of resolution and sensitivity.

GMR structure consist of generally a waveguide with a grating structure on top of it with which has RI supporting the resonance and on the other end generally a substrate is present providing the suitable conditions for resonance to happen and many times even helping to optimize it in some way or form. .

2 Theoretical Model

Considering a GMR structure consisting of a 1D line grating with period Λ on a planar waveguide of thickness 'd'. RI of the cover, waveguide and substrate are denoted as n_c , n_w & n_s respectively. n_w , n_c and n_s represent refractive index of waveguide, cover and substrate. we are considering TM polarized light which is incident at an angle θ_{inc} .

$$\phi = 2k_{c,w}d + \phi_{w,s} + \phi_{w,f} \quad (1)$$

Giving the value of total phase shift at the end of one round trip after which the diffracted order couples out of waveguide [1]. The first term is phase difference intoduced by optical distance, the second and third term are shifts due to total internal reflections at the respective medium junctions.

$$k_{c,w} = k_0(n_w^2 - n_{eff}^2)^{1/2} \quad (2)$$

n_{eff} is the effective waveguide index.

2.1 Azimuthal Angle

Generally GMR structures are mounted in a configuration where the grating vector lies on plane of incidence. In canonical mounting the substrate is rotated about the axis normal to its surface. This makes the diffracted order to deviate from the plane of incidence and lie on a cone. It is known that output GMR peak can be tuned by the use of azimuthal rotation. This occurs due to the change in propagation constant of wave coupled from the grating. In the configuration θ_{inc} is the angle between incident light and the axis normal to grating surface. ϕ_{inc} is the angle between the plane of incidence and the axis parallel to the grating vector \vec{K} which has a magnitude of $2\pi/\Lambda$. In Azimuthal rotation, the x,y,z coordinates of incident wave vector \vec{k}_{inc} can be expressed in terms of spherical polar coordinates as: [2]

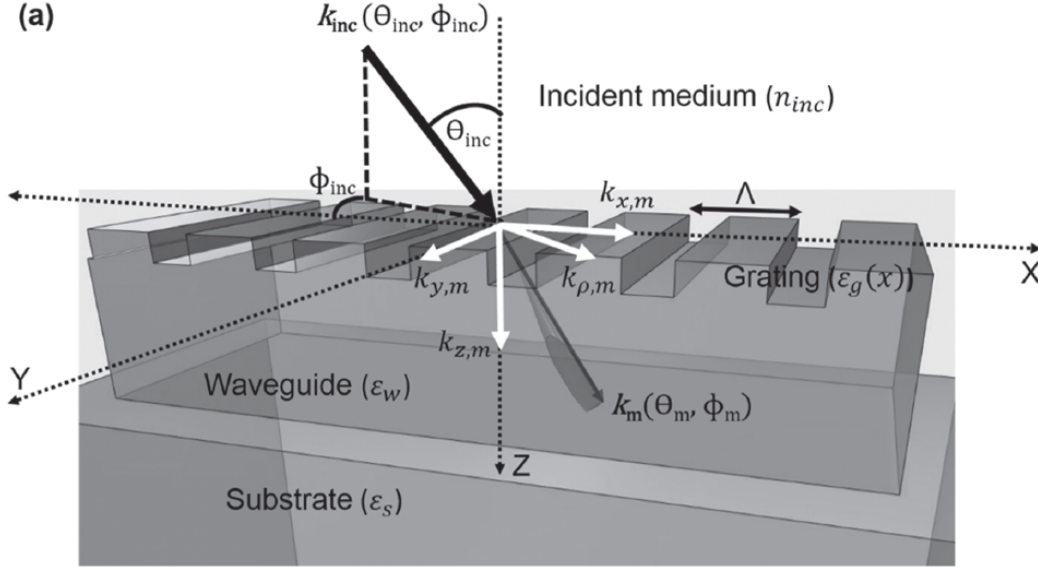


Figure 1: isotropic view of canonical mounting

$$k_{x,inc} = k_0 n_{inc} \sin \theta_{inc} \cos \phi_{inc} \quad (3)$$

$$k_{y,inc} = k_0 n_{inc} \sin \theta_{inc} \sin \phi_{inc} \quad (4)$$

$$k_{z,inc} = k_0 n_{inc} \cos \theta_{inc} \quad (5)$$

After diffraction all the diffracted order lie on a cone which has its axis perpendicular to grating vector and lie on the grating surface(y), implying that all have same y component and that component is equal to the y component of incident wave vector ($k_{y,m} = k_{y,inc}$). The x component changes according to phase matching diffraction condition, for m^{th} order: $k_{x,m} = k_{x,inc} - mK$.

in resonance the diffracted mode is coupled into the waveguide as a guided mode with a propagation constant ($\beta_m = n_{eff} k_0$) equal to grating surface component of diffracted wave vector \vec{k}_m giving the formula $\beta_m = \sqrt{(k_{x,m}^2 + k_{y,m}^2)}$

$$\beta_m = k_0 \sqrt{(n_{inc} \sin \theta_{inc})^2 - 2 n_{inc} \sin \theta_{inc} \phi_{inc} \lambda_0 / \Lambda + m^2 \lambda_0^2 / \Lambda^2} \quad (6)$$

Only certain wavelengths which satisfy the eigenvalue equations of waveguide, are guided through the waveguide. The expression for β_m works with both TM and TE

polarization. But the eigenvalue equations for TM and TE are different to find the GMR wavelength we need to solve for them separately. This provides the tunable wavelength filter function. But we used a more computational path for finding out the wavelength range.

2.2 TM polarization

Referring to the configuration with dominant field parallel to grating grooves as TE mode and perpendicular one as TM. Rigorous coupled wave analysis simulations show that the comparatively higher 'Q factor of GMR peak' and sharper phase response of TM mode higher than that of TE [3]. The fields which are at the interface of cover and waveguide in TE mode face less resistance while scattering into the far field as these fields at the interface are in phase, this leads to TE having lower Q factor hence lower sensitivity for phase detection. On the other hand TM mode scattering at interface is reduced by the destructive interference because of the fields at interface being antiphase. For these reasons we picked up with TM polarization in our analysis.

2.3 Wavelength Regimes

From eq.(6) we get the final equation for n_{eff} :

$$n_{eff} = \sqrt{(n_{inc}\sin\theta_{inc})^2 - 2n_{inc}\sin\theta_{inc}\phi_{inc}\lambda_0/\Lambda + m^2\lambda_0^2/\Lambda^2} \quad (7)$$

for the resonance to occur n_{eff} should satisfy the inequality:

$$\max\{n_s, n_f\} \leq n_{eff} \leq n_w \quad (8)$$

Solving this inequality will provide us the wavelength regimes for which guided mode resonance is possible under the presented circumstances. We opted to computationally find out the wavelength regimes by calculating every n_{eff} value and then putting it through a conditional representing the inequality. after fixing a variable of azimuthal angle we will be able to plot the regimes as wavelength vs incident angle graph. [4]

2.4 Phase shift by T.I.R.

When TIR happens there is no transmission of energy to the second medium. Considering only the TM mode the fresnel formulae are written in the following form giving reflectance and amplitude relation. i and t are subscripts for incident and transmitted.

$$R_{||} = \frac{\sin\theta_i\cos\theta_i - \sin\theta_t\cos\theta_t}{\sin\theta_i\cos\theta_i + \sin\theta_t\cos\theta_t} A_{||} \quad (9)$$

By solving the complex conjugate representation of the field using this and doing some more complex analysis we get the formulae for phase change due to total internal reflection. for TM mode (parallel): [5]

$$\tan \frac{\phi_{||}}{2} = -\frac{\sqrt{\sin^2\theta_i - n^2}}{n^2\cos\theta_i} \quad (10)$$

Here, $n=n_2/n_1$, . Now, for azimuthal angle zero and 0^{th} order diffracted wave we have $n_{eff} = n_{inc}\sin\theta_{inc}$. Using this, converting $\cos\theta_{inc}$ in terms of $\sin\theta_{inc}$ and renaming variables we get:

$$\tan \frac{\phi_{w,s}}{2} = -\frac{n_w^2}{n_s^2} \sqrt{\frac{n_{eff}^2 - n_s^2}{n_w^2 - n_{eff}^2}} \quad (11)$$

$$\tan \frac{\phi_{w,f}}{2} = -\frac{n_w^2}{n_f^2} \sqrt{\frac{n_{eff}^2 - n_f^2}{n_w^2 - n_{eff}^2}} \quad (12)$$

2.5 Resultant Phase

The Final resultant phase is calculated by solving the field equation of the final resultant complex wave which is formed by the interaction of all the different diffracted orders coming out of the waveguide and the 0th order reflected wave $R_0 = e^{i\omega t}$. The resultant wave is given by: where N is the number of round trips. [1]

$$E_r = e^{i\omega t} + e^{i(\omega t - \phi)} + e^{i(\omega t - 2\phi)} \dots + e^{i(\omega t - (N-1)\phi)} \quad (13)$$

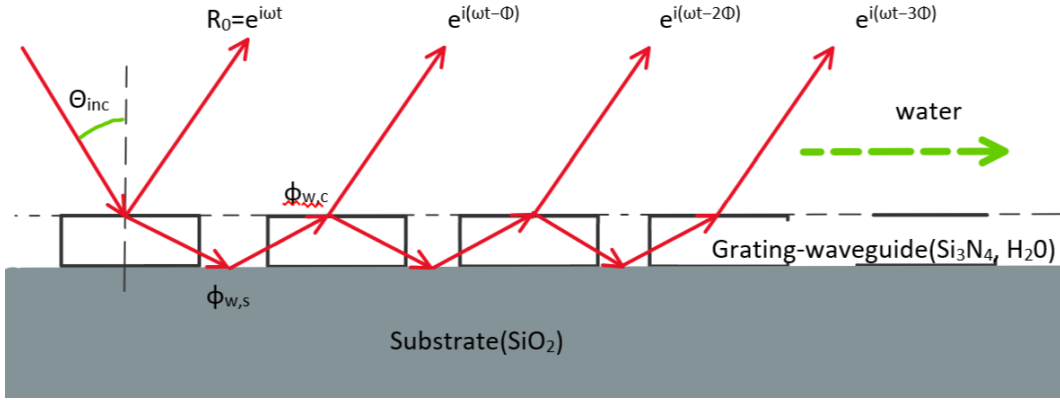


Figure 2: GMR diagram explaining the formation of complex resultant wave E_r

3 Results and discussion

We considered parameters of the experiment as, grating thickness is 150 nm, substrate is glass with RI 1.45, top layer is water covered with RI 1.331, grating period is 572 nm, fill factor is 75%, grating length is 500 μm . After taking into account these parameters we started to work towards plotting wavelength vs incident angle graphs with different azimuthal angles to find the wavelength regimes through the use of MATLAB. Grating covered by low refractive index substrates can also act as a waveguide layer if the phase matching conditions are matched. So even without the waveguide layer the GMR effect can occur, So the equations for the sample can be written as:

$$\phi = 2k_{c,w}d + \phi_{w,s} + \phi_{w,c} \quad (14)$$

The refractive index of equivalent waveguide is given by:

$$n_w = \frac{1}{\sqrt{\frac{f_H}{n_h^2} + \frac{1-f_H}{n_L^2}}} \quad (15)$$

Here, f_H is the fill factor and n_L , n_H are lower and higher refractive index, respectively. from here we calculated the number of round trips by using the grating length. we get n_w 1.744. Now, to find N, which is the number of round trips in total, we calculate by using the basic geometry of a waveguide fig(3). We focused on this with

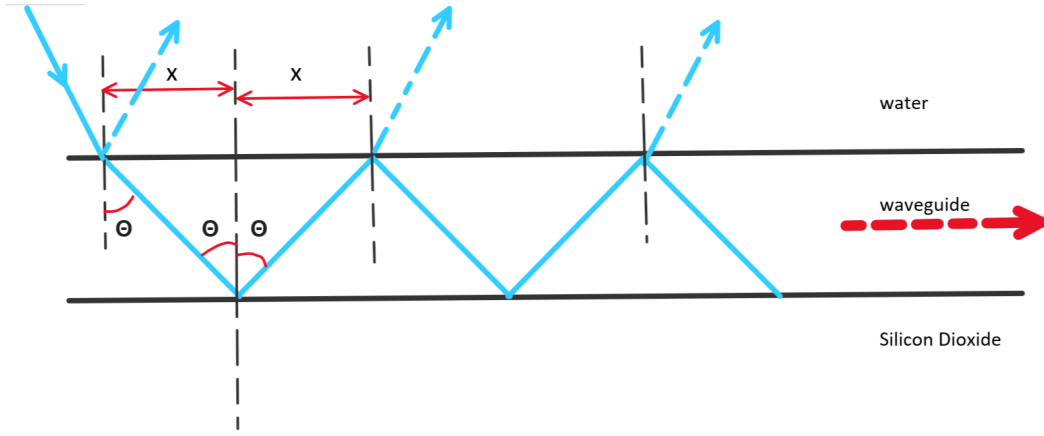


Figure 3: GMR diagram explaining the proof structure for finding number of round trips.

azimuthal angle as zero. we consider $2x$ as the length of one round trip and grating length divided by $2x$ gives us N .

$$\begin{aligned}
 n_{eff} &= n_w \sin \theta \\
 1.45 &< n_{eff} < 1.744 \\
 0.7816 &< \sin \theta < 1 \\
 0.8973 &< \theta < \pi/2 \\
 1.2532 &< \tan \theta < \infty \\
 \tan \theta &= \frac{x}{150} \\
 2x &= 300 \tan \theta \\
 2x &> 375.98 \text{ nm} \\
 N &< \frac{500 \mu\text{m}}{375.98 \text{ nm}} \\
 N &< 1329.85
 \end{aligned} \tag{16}$$

After calculating the further required parameters we plotted the wavelength vs incident angle graph which will provide us with the wavelength regimes by using the inequality eq.(8) which converts into $1.4 \leq n_{eff} \leq 1.744$ and eq.(7). we got the graph fig(4).

After getting the wavelength range for our mounting setup which was incident angle zero and azimuthal angle zero at $m=1$. We find that 855 nm is an acceptable wavelength for this setup as the wavelength regime shows it supports GMR in given conditions. From eq.(15) we set the value of N to 1000. All this is now used to calculate the total phase and phase difference with respect to minute changes in RI of water. We used matlab functions to add the complex equations and find out the resultant phase brought upon by the change in RI of the water. Plotted change in RI vs change in phase and RI vs phase for finding the sensitivity and then smooth the plot. Following are data points for the Delta RI vs delta phase graph tab.(1).

According to the fitting from fig(6), where the most steep change observed which is in between refractive index 1.336 and 1.337 is focused and fitted, the maximum possible sensitivity for this sample structure is $922 \pi \text{ RIU}^{-1}$. The change in phase with respect to micro changes in RI, along with this maximum sensitivity demonstrate the superiority of TM mode based phase sensing in GMR structure.

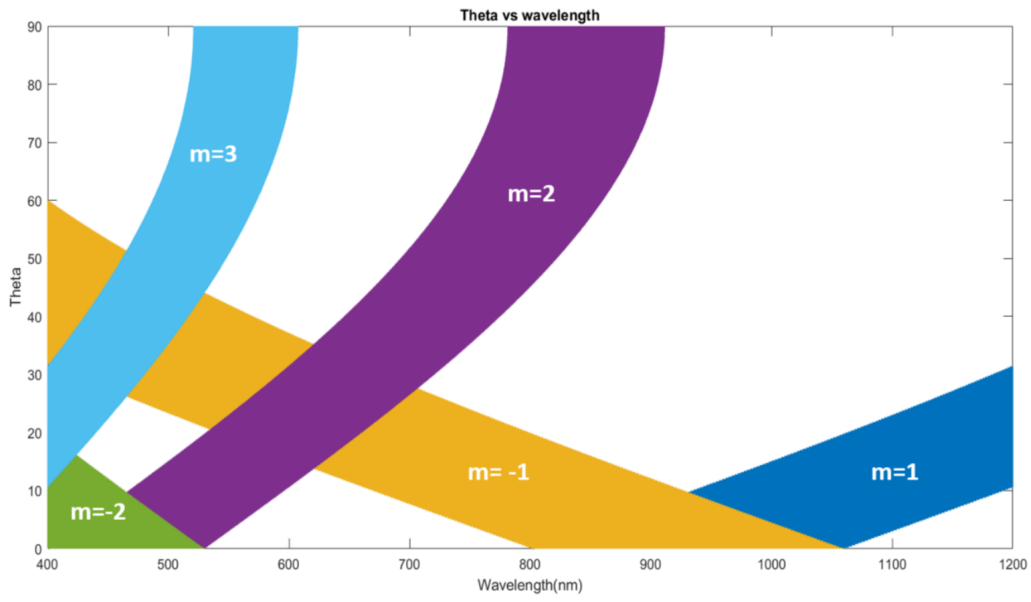


Figure 4: wavelength vs incident angle at azimuthal angle zero

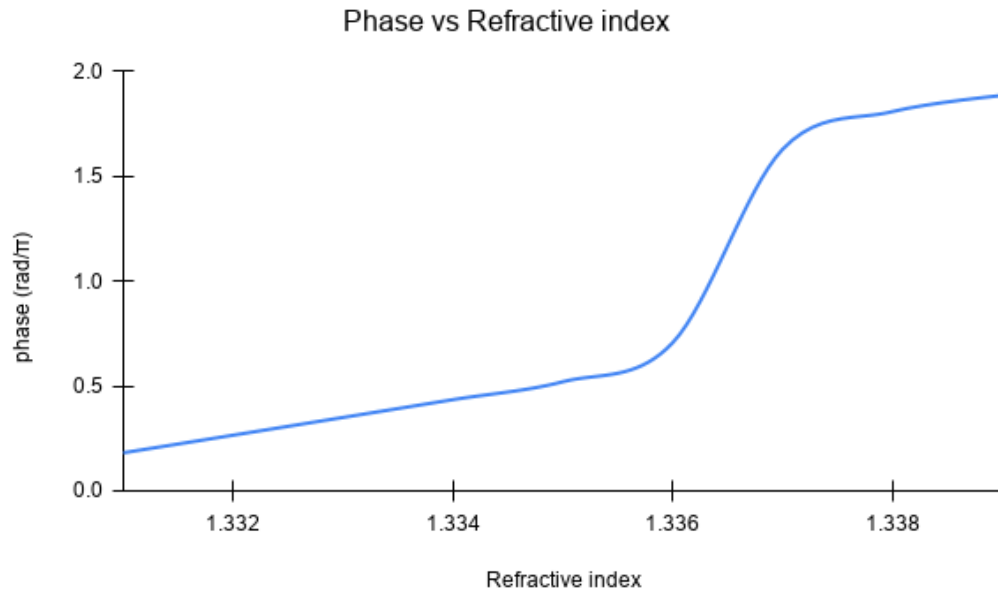


Figure 5: Total phase vs Refractive index of the cover

Wavelength vs incident angle plot represent different modes in which all corresponding modes with opposite signs and equal natural value meet at bottom of the curve.

Change in RI	Change in Phase [rad/ π]
0	0
0.001	0.08406099398
0.002	0.1685293243
0.003	0.2534087725
0.004	0.3387031772
0.005	0.5244164354
0.006	1.446654126
0.007	1.627115399
0.008	1.704109202

Table 1: Data points for delta RI vs delta Phase plot

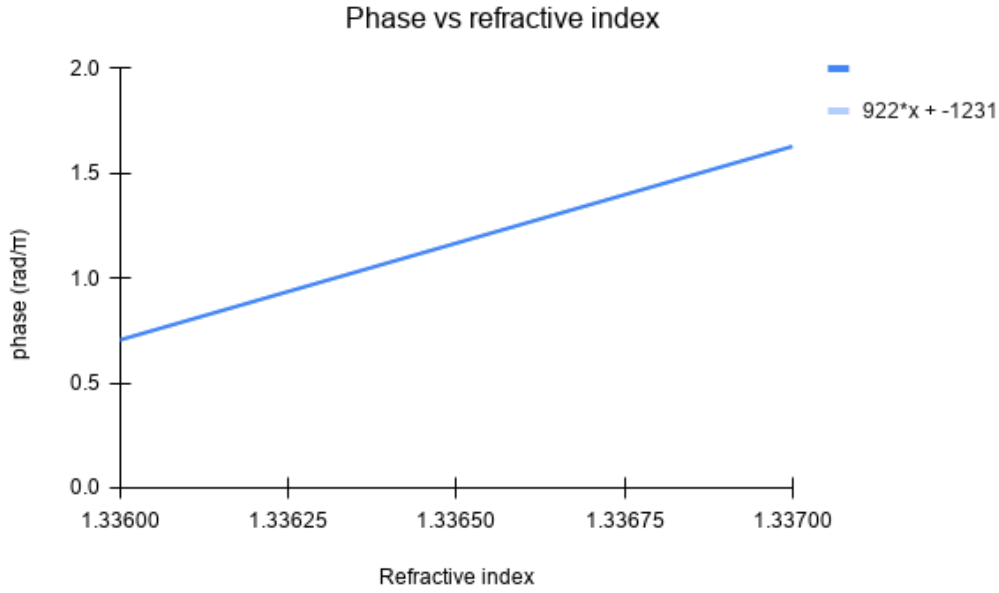


Figure 6: Change in phase vs change in refractive index, with fitting equation.

4 Conclusions

Demonstrated a analytical model producing maximum sensitivity of $S=922 \pi \text{ RIU}^{-1}$ with a GMR structure which included a grating with grating period 572 nm, thickness of 150 nm, substrate as glass, cover as water, fill factor of 75% and grating length is 500 μm . Employed analytical model under which configuration is of perpendicular incidence and azimuthal angle zero and wavelength 855 nm. In this model we employ the concept of phase sensitivity by finding out the 'wavelength regimes', under which GMR is allowed, governed by the present spacial configuration (incident angle and azimuthal angle) of the sample structure along with optical properties of the setup (RI of grating, etc.) and then using the sensitivity of GMR peak to measure the change in surrounding RI. We also presented the concept of wavelength tuning through azimuthal rotation. This allows us to highly optimize the usage of phase detection as a wide range of wavelength and spacial configurations which allow GMR to occur are unlocked.

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- [3] sabel Barth, Donato Conteduca, Christopher Reardon, Steven Johnson and Thomas F. Krauss, “Common-path interferometric label-free protein sensing with resonant dielectric nanostructures,” Barth et al. Light: Science & Applications (2020) 9:96.
- [4] S. S. Wang and R. Magnusson, “Theory and applications of guided-mode resonance filters,” APPLIED OPTICS / Vol. 32, No. 14 / 10 May 1993.
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by Navneet Singh

Submission date: 14-May-2021 09:22PM (UTC+0530)

Submission ID: 1586079277

File name: 2017PH10832_PYD411_ER.pdf (773.06K)

Word count: 2390

Character count: 11992



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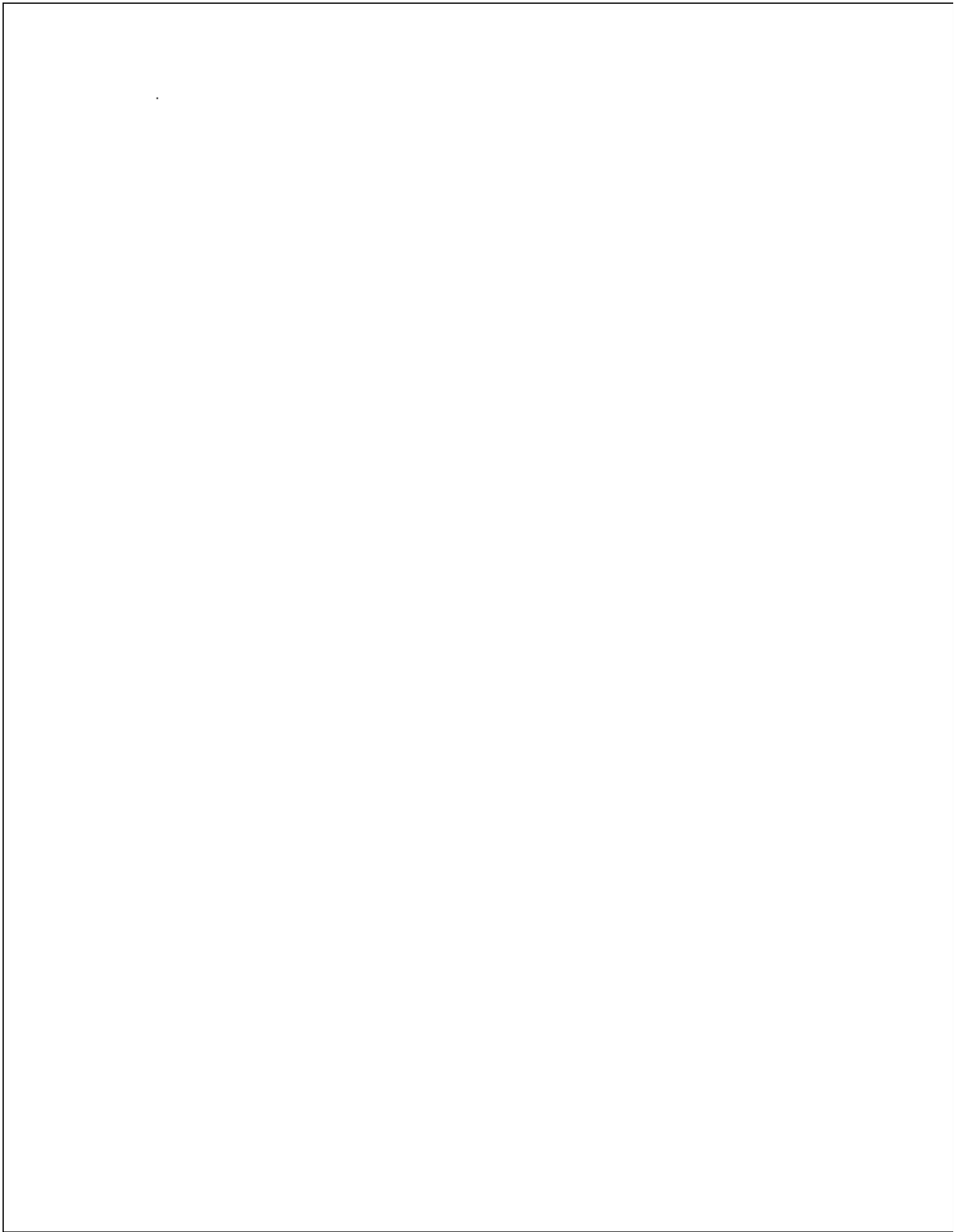
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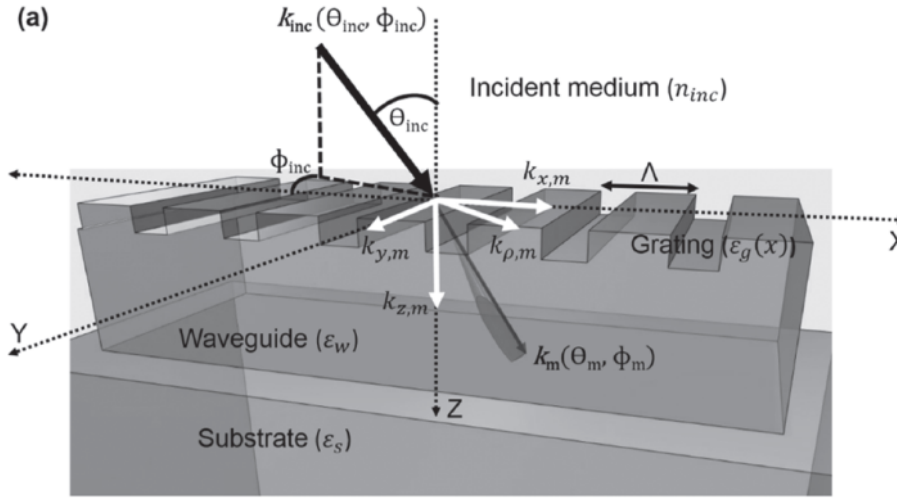


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The Final resultant phase is calculated by solving the field equation ⁴ of the final resultant complex ³ wave which is formed by the interaction of all the different diffracted orders coming out of the waveguide and the 0th order reflected wave $R_0 = e^{i\omega t}$. The resultant wave is given by: where N is the number of round trips. ¹

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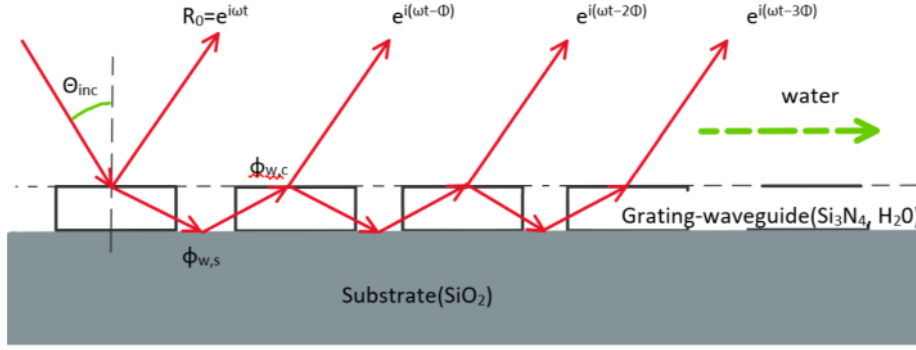


Figure 2: GMR diagram explaining the formation of complex resultant wave E_r

¹¹ 3 Results and discussion

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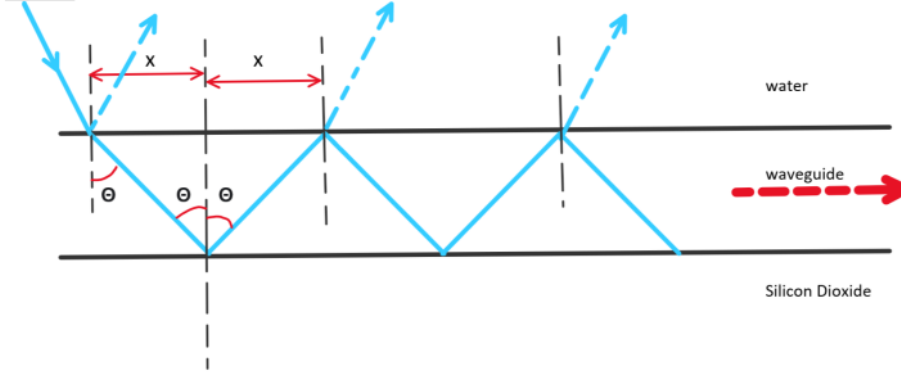


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 \end{aligned} \tag{16}$$

After calculating the further required parameters we plotted the wavelength vs incident angle graph which will provide us with the wavelength regimes by using the inequality eq. (8) which converts into $1.4 \leq n_{eff} \leq 1.744$ and eq. (7). we got the graph fig (4).

After getting the wavelength range for our mounting setup which was incident angle zero and azimuthal angle zero at $m=1$. We find that 855 nm is an acceptable wavelength for this setup as the wavelength regime shows it supports GMR in given conditions. From eq. (15) we set the value of N to 1000. All this is now used to calculate the total phase and phase difference with respect to minute changes in RI of water. We used matlab functions to add the complex equations and find out the resultant phase brought upon by the change in RI of the water. Plotted change in RI vs change in phase and RI vs phase for finding the sensitivity and then smooth the plot. Following are data points for the Delta RI vs delta phase graph tab. (1).

According to the fitting from fig (6), where the most steep change observed which is in between refractive index 1.336 and 1.337 is focused and fitted, the maximum possible sensitivity for this sample structure is $922 \pi \text{ RIU}^{-1}$. The change in phase with respect to micro changes in RI, along with this maximum sensitivity demonstrate the superiority of TM mode based phase sensing in GMR structure.

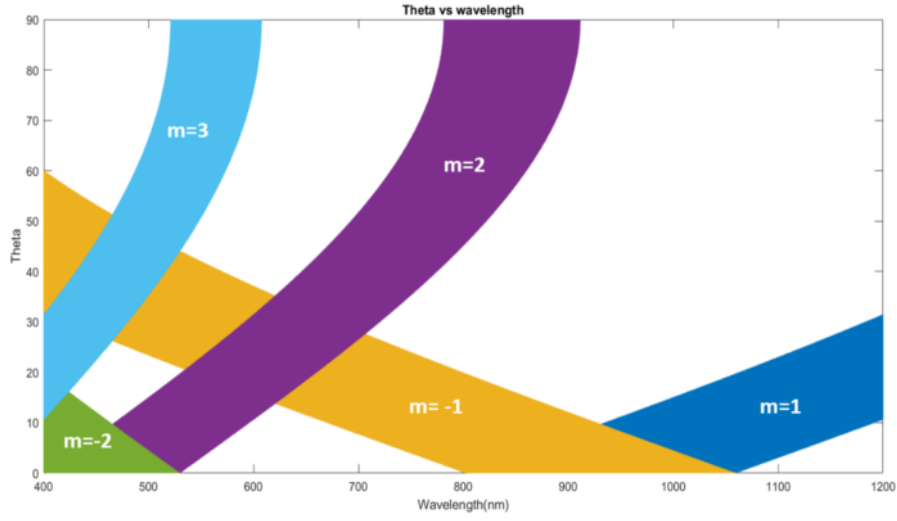


Figure 4: wavelength vs incident angle at azimuthal angle zero

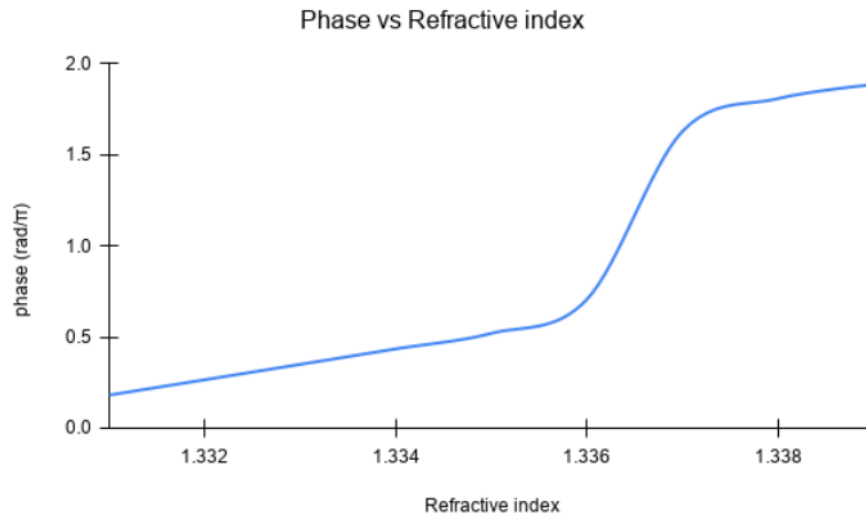


Figure 5: Total phase vs Refractive index of the cover

Wavelength vs incident angle plot represent different modes in which all corresponding modes with opposite signs and equal natural value meet at bottom of the curve.

Change in RI	Change in Phase [rad/ π]
0	0
0.001	0.08406099398
0.002	0.1685293243
0.003	0.2534087725
0.004	0.3387031772
0.005	0.5244164354
0.006	1.446654126
0.007	1.627115399
0.008	1.704109202

Table 1: Data points for delta RI vs delta Phase plot

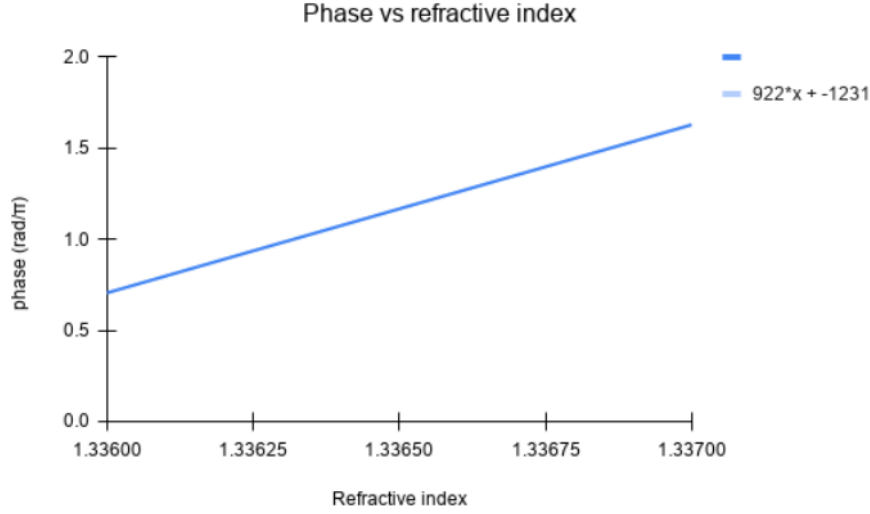


Figure 6: Change in phase vs change in refractive index, with fitting equation.

4 Conclusions

Demonstrated a analytical model producing maximum sensitivity of $S=922 \pi \text{ RIU}^{-1}$ with a GMR structure which included a grating with grating period 572 nm, thickness of 150 nm, substrate as glass, cover as water, fill factor of 75% and grating length is 500 μm . Employed analytical model under which configuration is of perpendicular incidence and azimuthal angle zero and wavelength 855 nm. In this model we employ the concept of phase sensitivity by finding out the 'wavelength regimes', under which GMR is allowed, governed by the present spacial configuration (incident angle and azimuthal angle) of the sample structure along with optical properties of the setup (RI of grating, etc.) and then using the sensitivity of GMR peak to measure the change in surrounding RI. We also presented the concept of wavelength tuning through azimuthal rotation. This allows us to highly optimize the usage of phase detection as a wide range of wavelength and spacial configurations which allow GMR to occur are unlocked.

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