Response to Reviewer 2 Comments

We would like to thank the reviewer for your positive feedback and constructive suggestions on our Manuscript ID: nanomaterials-510144: “Guided mode resonance sensors with optimized figure of merit”. In the revision, we carried out extensive studies based on those feedback and suggestions. In the following pages, we list point-by-point response to reviewers’ comments.

For your convenience, we provide this MANUSCRIPT REVISIONS DETAILS with the reviewers’ comments in black. All responses made to the text are in RED color here.

REVISIONS DETAILS:

“The manuscript by Xiang et al. reports evaluations of figure of merit in guided mode resonance (GMR) sensors. The authors employed an analytical model and a finite element analysis method to explore the GMR effects in the optical sensors. By this, they systematically explored the geometrical dependence of the sensitivity and the resonant linewidth for both waveguide-grating and grating-waveguide GMR configurations. As a result, it was found that the optimal grating period is linearly correlated to the groove depth.

The results reported, in particular Figs. 5c and 5d, may be useful in developing practical GMR sensors, and thus will be good contribution to the field. However, the paper is not organized well and requires extensive revision before it can be published in Nanomaterials. I would consider recommendation of the publication after the authors addressed the following points:”

Point 1: Most of the sentences in 3.2 is quite similar to those in 3.1. Also, Figs. 1 and 3 together with the corresponding discussions are almost the same to each other. Meanwhile, it is very difficult to find any reasons to work on the two situations. The authors must first explain the point to study the angular and wavelength shifts, and then try not to repeat the same explanations/discussions on the results.

Response 1: Using Equation 2 and 3 to calculate phase shift curve in waveguide layer for angular and wavelength resonance, respectively, we can obtain the following Figure S1. The x axis represents propagation angle in waveguide layer, y axis stands for phase shift. Angular resonance and wavelength resonance have similar phase shift curve, as they have similar waveguide parameters. Although the grating period is different, it only influences the left side of Equation 2 and 3, as the purple and gray curves shown in Figure S1. So, we use the same way to discuss these two situations.
Figure S1. Phase shift curve in waveguide layer at different propagation angle, (a) angular resonance, (b) wavelength resonance.

To emphasize the points for angular and wavelength resonance, we add some statements to describe their difference. In section 3.1, the following description is added to point the angular resonance: “For an angular interrogation technique, a monochromatic light source, such as a He–Ne laser, is typically used to measure the GMR effect in this case” (in Page 3, Line 102). Following sentences are added at the beginning of Section 3.2: “The most common detection technique for GMR sensors is the wavelength shift-tracking method. A broadband light source is used, such as an LED light and white light source” (in Page 6, Line 182).

Besides, we have modified the repeated discussions/explanations. The main contents are focused on the comparison of results between Section 3.1 and 3.2, and try to explain their underlying physics. The details are as the following:

“The electric field distributions for both TE and TM polarization were simulated to further explain the previous results and are shown in Figure 3g–j. Compared to Figure 1g–j, similar results can be achieved here. For TE mode, most of the evanescent field energy exists in the waveguide layer, and thus the sensing performances were affected. TM cases have a larger light-matter interaction region in the cover medium, and more light is strongly confined (the maximum electric intensity up to 3.61×10^6 V/m), making it more suitable to achieve better performances in biosensing.” (in Page 7, Line 201)

“Combining these results with those of Section 3.1, TM polarization has better results for both angular and wavelength resonance, although different detection methods were used. This phenomenon can be explained in two respects: first, TM polarized modes have a larger phase shift length at the resonance point compared to TE modes, resulting in higher sensitivity, as shown in Figure 4. The red and blue curves represent the TM polarization phase shift in the waveguide layer at different surrounding \( n_c \). Yellow and green curves represent the TE polarization phase shift at different surrounding \( n_c \). The label \( d_{wg} = 60 \) nm (purple curve) and \( d_{wg} = 90 \) nm (gray curve) represent the calculated results coming from left side of Equation 2 and 3 (called structure relation [35]). The intersection points of the structure relation curve and phase shift curve represent the points of resonant condition, where the GMR effect occurs. The length between two intersection points is proportional to resonant angle or wavelength shift. Therefore, a larger phase change length at different \( n_c \), results in greater sensitivity. In Figure 4, the TM polarization has a larger phase change length compared to the TE mode, when the \( d_{wg} \) was 90 nm. Second, the coupling-loss coefficient for a TM polarization was smaller than that for the TE polarization, resulting in a narrow linewidth [46]. Besides, the \( d_{wg} = 90 \) nm (purple curve) case has a larger phase shift length than the \( d_{wg} = 60 \) nm (gray curve) condition for TM
polarization. This also explains why a higher sensitivity was obtained for the case where $d_{wg} = 90$ nm, as shown in Figure 1f and Figure 3f.” (in Page 7, Line 212)

**Point 2:** Section 3.3 discusses optimal sensor performance of “waveguide-grating” GMR structures. This is quite puzzling as the preceding sections are about “grating-waveguide” configurations. The authors need to make it clear why they did not examine the sensor structure optimizations of their “waveguide-grating” GMR structures and instead worked on the “grating-waveguide” GMR sensors.

**Response 2:** The “grating-waveguide” GMR structures have been optimized in section 3.1 and 3.2. For instance, in Section 3.1, a maximum FOM of 5709 was achieved when $d_g$ was 10 nm and $d_{wg}$ was 90 nm ($d$ set 100 nm) for TM polarization. The design rule for “grating-waveguide” GMR sensors to achieve optimized FOM is shown in Page 5, Line 170: “For optimizing FOM of “grating-waveguide” GMR sensors, a high value region of sensitivity should be evaluated first and then $d$ should be maintained near this value. Finally, by fabricating a shallower grating depth, a higher sensitivity and narrower linewidth will be achieved, resulting in an excellent FOM.”

**Point 3:** On page 5, “a shallower $d_g$ facilitates a narrower linewidth” of Line 151 cannot be straightforwardly assessed from their results. This is because the authors fixed $d$ in Fig. 1. They should fix $d_{wg}$ and vary $d_g$ to prove this assertion.

**Response 3:** Because ref [46] had verified that a shallow grating depth will make the linewidth smaller, and similar results are obtained here, thus we directly used this conclusion here. To prove this assertion, under same $d_{wg}$ value, different $d_g$ is chosen to calculate the corresponding results, as shown in Table S1.

<table>
<thead>
<tr>
<th>$d_g$ (nm)</th>
<th>$d_{wg}$ (nm)</th>
<th>FWHM (degree)</th>
<th>S (degree/RIU)</th>
<th>FOM</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>90</td>
<td>0.0011</td>
<td>25.298</td>
<td>22998.182</td>
</tr>
<tr>
<td>10</td>
<td>90</td>
<td>0.0045</td>
<td>25.692</td>
<td>5709.311</td>
</tr>
<tr>
<td>20</td>
<td>90</td>
<td>0.0165</td>
<td>26.136</td>
<td>1584.000</td>
</tr>
<tr>
<td>30</td>
<td>90</td>
<td>0.0351</td>
<td>26.432</td>
<td>755.200</td>
</tr>
<tr>
<td>40</td>
<td>90</td>
<td>0.0581</td>
<td>26.591</td>
<td>458.465</td>
</tr>
</tbody>
</table>

From Table S1, we can clearly find that a shallower $d_g$ results in a narrower linewidth.

**Point 4:** The authors need to explain why different grating periods were used in Secs. 3.1 and 3.2.

**Response 4:** In Section 3.1, the grating period of 280 nm can suitable for oblique incidence at a relative larger incident angle, when the 633 nm monochromatic light was used as light source. If we still set the grating period at 280 nm for normal incidence, it leads to resonant wavelength around 400 nm region. However, many white light sources can’t produce a stable output light near this wavelength range. The limitation of light sources may be able to block GMR effect. On the other side, grating period at 410 nm can lead to resonant wavelength around 600 nm, which is suitable for experiments. So, for realistic consideration, the different grating periods were used in Sections 3.1 and 3.2.
Point 5: The manuscript only shows the simulation results without physical explanations. For instance, the linear relation in Fig. 5 better be discussed from physics points of view. Moreover, it is noted several times that “more energy was confined in the structure, thus decreasing the resonant linewidth” and “the electric field is mainly stored in the waveguide layer” without any descriptions of the underlying physics.

Response 5: The linear relation in Figure 5 (Figure 5 has been changed to Figure 6 in revised manuscript) is a series optimized results which obtained from different grating periods. Follow description is added in the revised manuscript (in Page 10, Line 279). “The point of these optimized FOM is that a narrow resonant linewidth occurred abruptly, as shown in Figure 5c,e. Norton et al. investigated linewidth of “waveguide-grating” GMR structure through coupled-mode theory [47]. Briefly, the angular and wavelength linewidth is proportional to coupling loss coefficient, and the coupling loss is determined by the overlap of the bound mode and the radiation mode within the film layer. At higher depths, the orthogonality of the two modes decrease the overall magnitude of the coupling loss, resulting in a narrow resonant linewidth. In our work, similar resonant linewidth change phenomenon can be found in Figure 5c,e. Although Norton et al. just investigated one grating period, it can be predicted that different grating periods have their own grating depths, where the narrow resonant linewidth occurs abruptly.”

The sentences, “more energy was confined in the structure, thus decreasing the resonant linewidth” and “the electric field is mainly stored in the waveguide layer”, can be explain as follow: “this result can also be proven by referencing [46], because the grating groove depth controls the coupling-loss coefficient in an exponential manner, thus the coupling-loss coefficient tends to be smaller as $d_g$ decreases” (in Page 3, Line 136).

Point 6: Significant figures should be corrected in Fig. 5 and Tab. 3. There are too many digits.

Response 6: We have removed redundant data in Figure 5 (Figure 5 has been changed to Figure 6 in revised manuscript) and Table 3, according to the reviewer’s advice.

Point 7: Abbreviation FEM is not for “finite element” but for “finite element analysis method”.

Response 7: We have changed “FEM” to “FEA”, according to ref [45].

Point 8: English writing needs to be improved throughout the manuscript.

Response 8: The manuscript has undergone English language editing by MDPI. And the details are marked in the revised manuscript.