ROMANIAN JOURNAL OF INFORMATION SCIENCE AND TECHNOLOGY
Volume **27**, Number 2, 2024, 207–216

Theoretical Studies of Intensity and Phase Based Surface Plasmon Resonance Sensors

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Abstract. In this work are presented the numerical results of reflectvity and phase dependence on the incidence angle for SPR configurations based on fused silica and BK7 substrate for various wavelengths from visible range. We have also determined the external angle of incidence on a right angle prism for optimal SPR sensitivity both for intensity and phase measurements.

Key-words: Abeles matrices method, sensing, surface plasmon resonance.

1. Introduction

The detection of small variations in the refractive index of media by means of the *surface plasmon resonance* (SPR) effect is a technique that was developed a few decades ago [1] and is now widely used thanks to its ability to perform labelling and measurements in real time, free from biochemical interactions. The most used configuration, which is also employed in SPR detection, is the so-called ”Kreschmann configuration” [2] which consists of a prism with a thin metallic film deposited on one of its surfaces. A (bio)chemical analyte with a refractive index to be determined is deposited on the outer part of the metal film. A low cost and simple way to realize an SPR sensor is to use a configuration based on a fixed angle of incidence and a fixed wavelength for the direct measurement of the intensity or phase of the reflected beam exiting from the prism. Even if this configuration is more simple than the ones based on angular or spectral interogation, it is necessary to find the condition of the optimal sensitivity (the maximal variation of the sensor response over the analyte refractive index variations). The condition can be determined from the analysis of the SPR response - the change of the intensity or phase with the internal incidence angle on glass-metal interface. The regions where the SPR response has the steepest variation are the best suited regions to set the internal incidence angle and subsequently the fixed external angle of incidence for a given wavelength.

In this work the SPR responses in intensity and phase for various configurations are calculated and the information regarding the optimal internal incidence angle will be used to calculate the value of the fixed external incidence angle. The results presented here will be further employed for experiments with SPR sensor working in intensity and/or phase interrogation.

2. Theoretical analysis

The proposed sensor configuration composed by a right angle prism with a slide having a reflective Cr/Au layer at the interface with the analyte.is shown in Fig. 1. The prism and the glass slide could be from different materials, which will increase the flexibility of the studied configuration. This is also close to the real cases when the glass slide with metal layer and microfluidic circuits filled with analyte will be attached via an index matching fluid on the prism. The ray trace into the prism and slide with the external incidence angle and the internal incidence angle is also represented in Fig. 1. Here, ρ is the external incidence angle, where for practical purposes, this was defined with respect to the horizontal axis. Also, the internal incidence angle ω_{slide} is defined with respect to normal direction to the glass slide/metal layers interface.

The intensity and phase response is studied for various wavelengths, and two *refractive index* (RI) values of the analyte (*e.g.*, 1.33 and 1.36). Two different substrate materials, BK7 with a refractive index of approximately 1.51 and fused silica with a refractive index of approximately 1.45 are considered. The exact refractive index values corresponding to the wavelengths of the two materials are given in [3]. For the sensitive layer, a Cr/Au metal sandwich was chosen, and the refractive index values for the two materials are derived from ref. [4] for Cr and ref. [5] for gold.

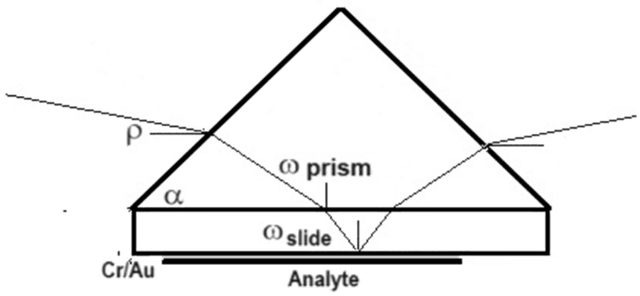

Fig. 1. Configuration of the SPR sensor with external incidence angle.

To analyze the numerical response, the Cr/Au metallic layers have thicknesses of 10 nm for chromium and 40 nm for gold. In order to obtain numerical results as close to reality as possible, it has been employed refractive index values from literature for metallic layers with thicknesses almost equal to those used in this analysis.

The response of the SPR sensor to different values of the medium refractive index has been obtained using a code written in C++ software based on Abeles matrices method as presented in [6]. This method allows to evaluate the intensity and phase change of the reflected/transmitted radiation for a multilayered structure by considering the wavelength, angle of incidence in superstrate (the glass slide), its refractive index, the complex refractive index of the metallic layers and their thickness and the refractive index of the substrate - the analyte. In the following, there are presented the results regarding the variation in reflected intensity (reflectivity) and phase with internal incidence angle on slide/metal interface - internal angle ω_{slide} shown in Fig. 1. The SPR response in intensity and phase depends strongly on radiation wavelength, substrate type and analyte refractive index. The results regarding the SPR response in intensity presented here were also presented in [7]. For all SPR responses in intensity and phase presented in this present work, the solid line and the broken line represents the SPR response for the analyte RI 1.33 and 1.36. respectively.

For the numerical analysis carried out at the wavelength of 635 nm shown in Figs. 2a and 2b, it is found that a variation of the SPR response can be used for the development of sensors if the substrate is BK7. If the analyte RI is around 1.33, as one can see from Fig. 2a., the largest variation of the SPR response in intensity is around 70 degrees, and if the analyte RI is around 1.36, the SPR response in intensity has the largest variation for 75 degrees of internal incidence angle. Also from SPR response in phase represented in Fig. 2b we notice that the largest variation is for 73 degrees in the case of analyte RI 1.33. If the analyte RI is centered around 1.36, the largest variation is for the 78 degrees internal angle.

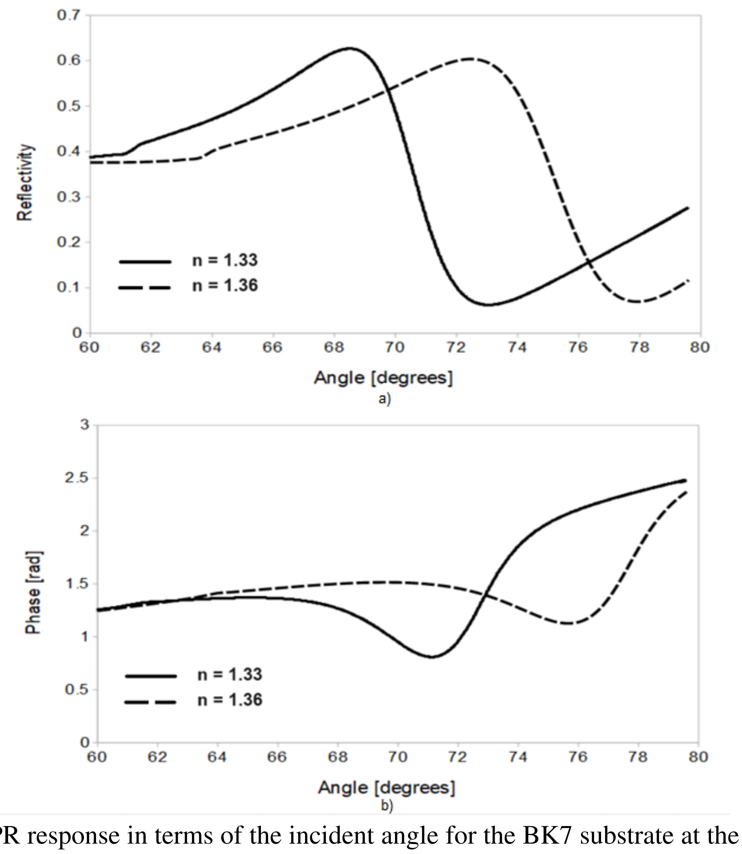

Fig. 2. The SPR response in terms of the incident angle for the BK7 substrate at the wavelength 635 nm. a) in intensity; b) in phase.

In the case of the 670 nm wavelength, strong variations of the SPR response have been obtained for both types of substrates considered, as is shown in Figs. 3 and 4. The results obtained for the BK7 substrate are better compared to the results obtained for the fused silica substrate. These qualitative differences are more significant if the analyte RI is 1.36. We notice from Fig. 3a that the largest‘variation of SPR in intensity with internal angle of incidence is at 68 degrees for analyte refractive index 1.33 and at 73 degrees for analyte refractive index 1.36, respectively. From Fig. 3b one can notice that the largest‘variation of SPR in phase with internal angle of incidence is at 71 degrees for analyte refractive index 1.33 and at 75 degrees for analyte refractive index 1.36, respectively.

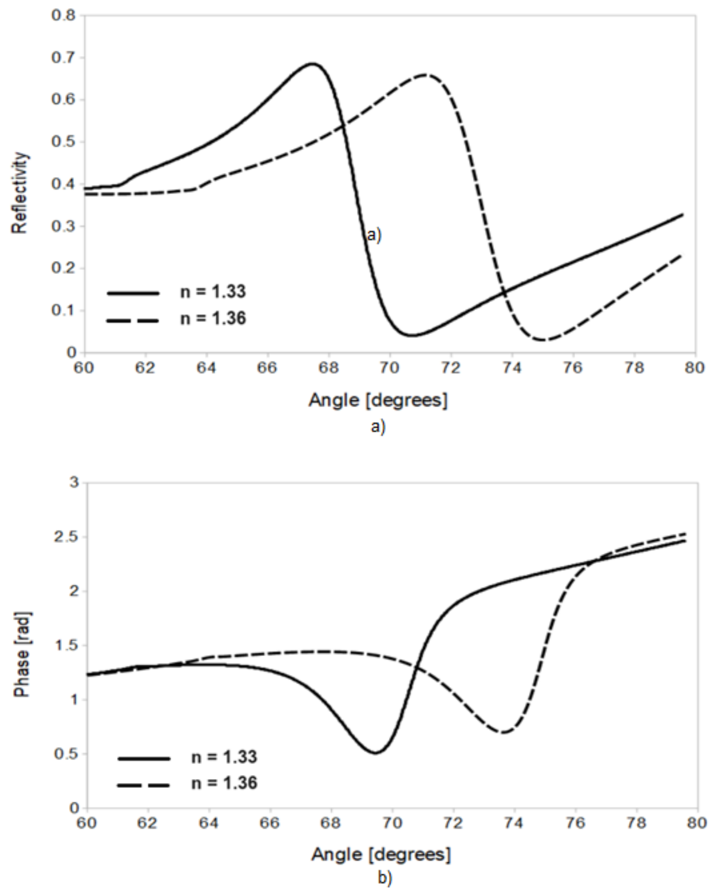

Fig. 3. The SPR response in terms of the incident angle for the BK7 substrate at the wavelength 670 nm. a) in intensity; b) in phase.

From Fig. 4a one can notice that the greatest variation of SPR response is obtained for internal angles centered at 75 degrees if analyte refractive index is 1.33 and 82 degrees if the analyte refractive index is 1.36, respectively. In the case of SPR response in phase represented in Fig. 4b, its largest variation is at 77 degrees (analyte RI =1.33) and 87 degrees (analyte RI=1.36).

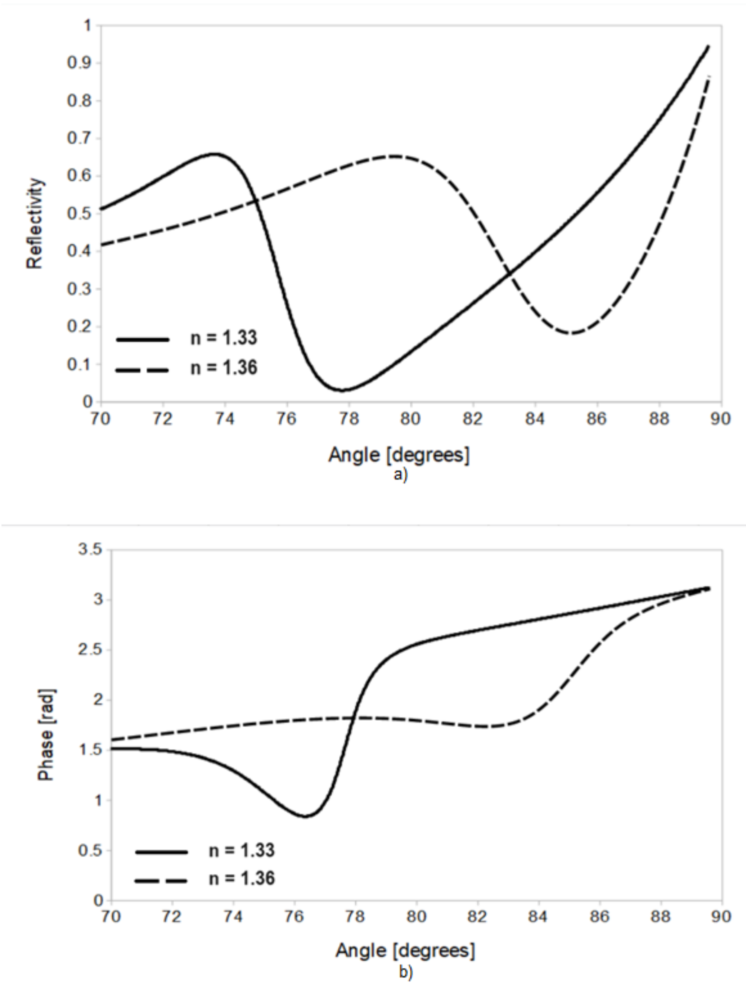

Fig. 4. The SPR response in terms of the incident angle for the fused silica substrate at the wavelength 670 nm. a) in intensity; b) in phase.

For 780 nm wavelength, promising results have been obtained regarding the SPR responses in intensity and phase, for both types of substrates, regardless of the value of the refractive index of the analyte selected from the range of interest. For the BK7 substrate, this can be seen in Fig. 5a for SPR response in intensity and in Fig. 5b for SPR response in phase. The steepest response is obtained at internal angles centered at 66 and 69 degrees for analyte RI 1.33 and 1.36, respectively, as one can see from Fig. 5a. In the case of SPR respone in phase, the steepest response is obtained at 67 degrees (analyte RI = 1.33) and 71 degrees (analyte RI = 1.36) as one can see from Fig. 5b.

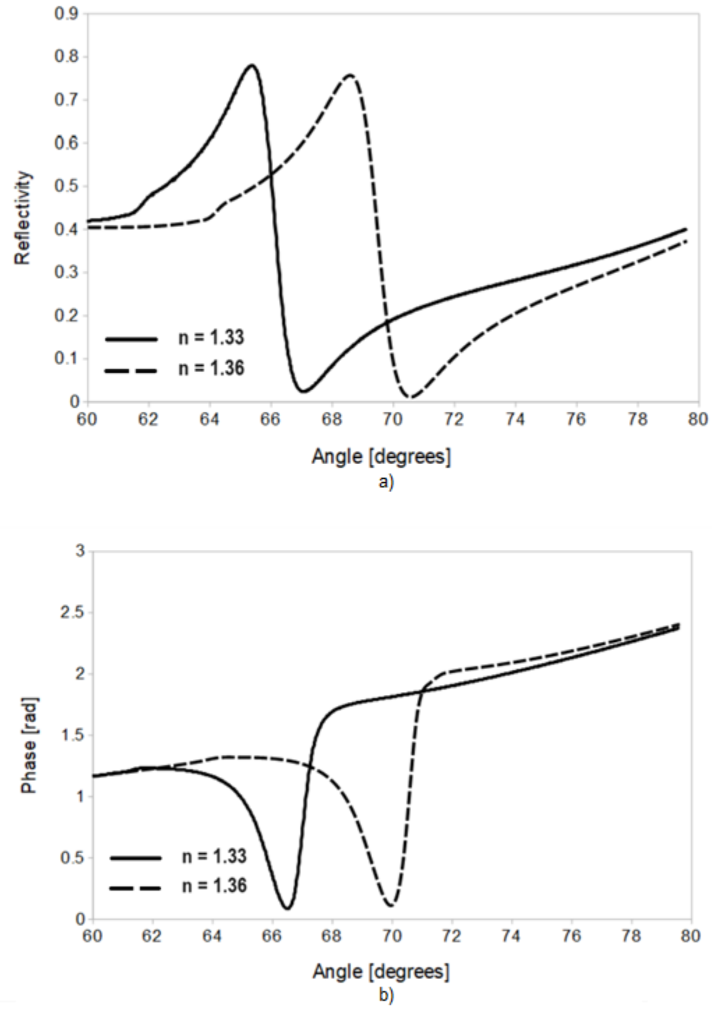

Fig. 5. The SPR response in terms of the incident angle for the BK7 substrate at the wavelength 780 nm. a) in intensity; b) in phase.

Similarly, the good results are obtained when the substrate is fused silica as illustrated in Fig. 6. In the case of SPR response in intensity represented in Figura 6a, the largest variation are found at 72 degrees if the analyte RI is 1.33 and at 77 degrees if the analyte RI is 1.36. In the case of SPR response in phase represented in Fig. 6b, the largest variation is obtained for 73 degrees if the analyte RI is 1.33 and for 78 degrees if the analyte RI is 1.36.

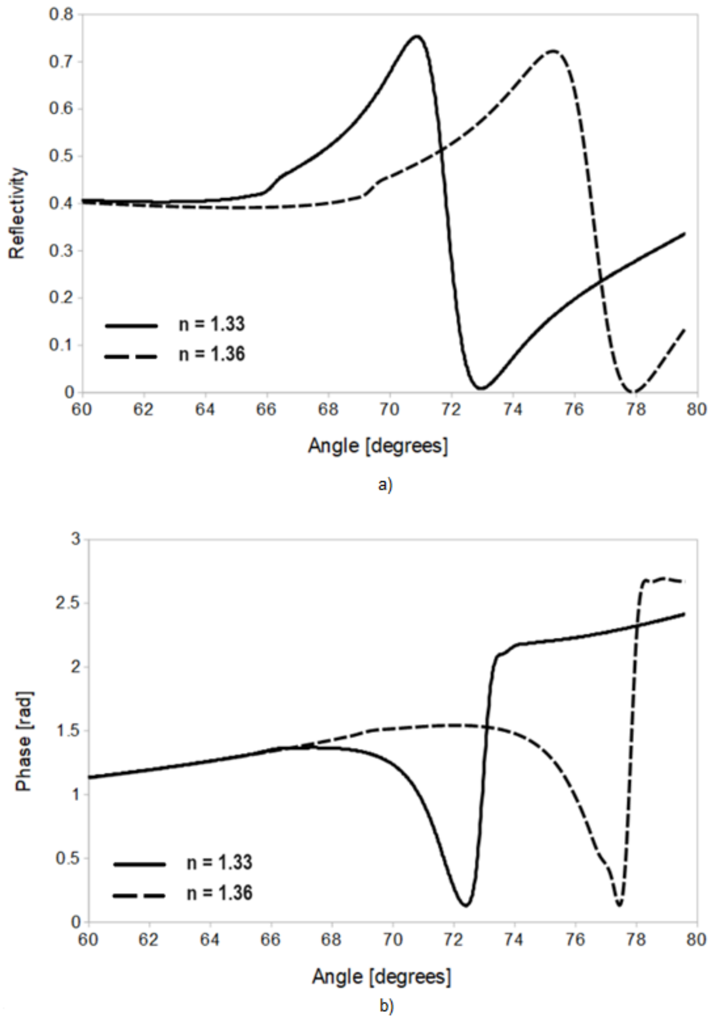

Fig. 6. The SPR response in terms of the incident angle for the fused silica substrate at the wavelength 780 nm. a) in intensity; b) in phase.

The external incidence angle ρ represented in Fig. 1 can be adjusted so the internal angle ω_{slide} presented in the same figure would have the value corresponding to the largest response variation. In order to obtain the relation between the external incidence angle and the internal angle, the expression presented in [8] eq. (3) has been used to deduce the value of ω_{prism} also represented in Fig. 1. The relation between the angles ω_{prism} and ω_{slide} can be deduced from the well known Snell law.

Four scenarios have been considered regarding the materials for prism and the glass slide, respectively, taking in account only two materials, BK7 and fused silica, noted further as FS. Thus, for the first case we have BK7 for prism, BK7 for slide, then the second case is FS (prism)/BK7 (slide), the third case is FS (prism)/ FS (slide) and the last case is BK7 (prism)/FS (slide). In the Fig. 7 is presented the dependence of internal angles on the external incidence angle for the all cases. A right angle prism with angle α from Fig. 1 equal to 45 degrees is considered, since this prism type from BK7 or FS materials are distributed by commercial vendors. It should be noted that in the case of BK7 prism and FS slide it could appear total internal reflection at the interface BK7/FS. This can be viewed in Fig. 7 when the internal angle approaches 90 degrees for lower values of the external incidence angle.

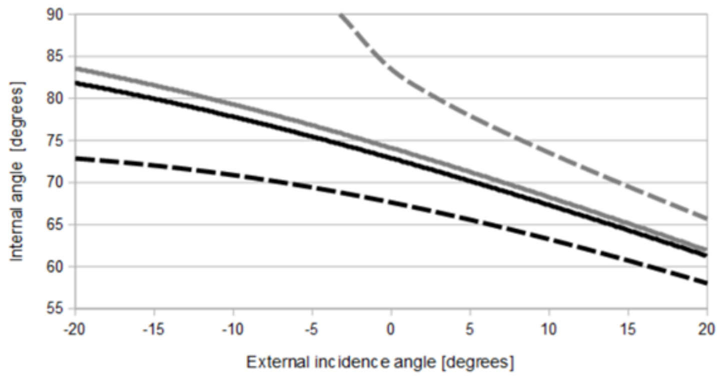

Fig. 7. The internal angle dependence on the external incidence angle. Case BK7 / BK7 (black line); Case FS /BK7 (dashed black line); Case FS / FS (gray line); Case BK7 /FS (dashed gray line).

Table 1. The SPR and external angle for various parameters

Wavelength nm	Prism	Slide	Response	Internal angle /**external angle** (medium RI))
635	BK7	BK7	Intensity	70/ **5** (1.33) 75/– **5** (1.36)
			Phase	73/ **0** (1.33) 78/ – **10** (1.36)
635	FS	BK7	Intensity	70/ – **7** (1.33) 75/ <– **20** (1.36)
			Phase	73/ < – **20** (1.33) 78/ <– **20** (1.36)
670	BK7	BK7	Intensity	68/ **6** (1.33) 73/ **0** (1.36)
			Phase	71/ **3** (1.33) ... 75/ – 5 (1.36)
670	FS	BK7	Intensity	68/ – **1** (1.33) ... 73/ – **20** (1.36)
			Phase	71/ – **11** (1.33) ... 75/ < – **20** (1.36)
670	FS	FS	Intensity	75/ – **2** (1.33) ... 82/ – **18** (1.36)
			Phase	77/ – **6** (1.33) ... 87/ < – **20** (1.36)
670	BK7	FS	Intensity	75/ **8** (1.33) 82/ **1** (1.36)
			Phase	77/ **6** (1.33) ... 87/ – **2** (1.36)
780	BK7	BK7	Intensity	66/ **12** (1.33) ... 69/ **6** (1.36)
			Phase	67/ **10** (1.33) ... 71/ **3** (1.36)
780	FS	BK7	Intensity	66/ **4** (1.33) ... 69/ – **4** (1.36)
			Phase	67/ **2** (1.33) ... 71/ – **10** (1.36)
780	FS	FS	Intensity	72/ **4** (1.33) ... 77/ – **6** (1.36)
			Phase	73/ **2** (1.33) ... 78/ – **8** (1.36)
780	BK7	FS	Intensity	72/ **12** (1.33) ... 77/ **6** (1.36)
			Phase	73/ **10** (1.33).... 78/ **5** (1.36)

In the Table 1 the optimal external incidence angle and the corresponding internal angle are listed for intensity or phase response considering various cases of prism and slide materials and the refractive index of the surrounding medium. The optimal external angle has been derived using SPR response curves in order to find the internal angle for the steepest response variation. The data represented in Fig. 7 has been used to set the correspondence from internal angle to the external incidence angle.

3. Conclusions

In this work numerical simulations on the intensity and phase response of the reflected radiation of an SPR sensor has been performed in terms of the environment refractive index.

The analysis made at the wavelengths 635 nm, 670 nm and 780 de nm leads to the conclusion that promising results can be obtained for the wavelengths 635 nm, 670 nm and 780 nm in the case of the glass BK7 substrate. In the case of the fused silica substrate we obtained good results for the wavelengths of 670 and 780 nm.

It is important to mention that the best results for fused silica are obtained at 670 nm radiation wavelength if the environment refraction index has its values close to 1.33. If the environment refractive index has a value close to 1.36, the SPR response does not have sharp variation characteristics.

The best SPR responses, with sharp variations for both values of the analyte refractive index and substrates types is obtained at 780 nm wavelength.

In order to obtain practically a SPR sensor based on intensity or phase response, it is necessary to know at least aproximately the internal angle range where one can obtain the greatest sensitivity and susequently the required external incidence angle range. It is highly reccomended to have the values of external incidence angles as lower as possible (the input and the exit beams should be almost parallel with the prism base). From the Table 1 one can notice that in the most cases the absolute values of the external incidence angle are lower than 10 degrees. This analysis is valid when the refractive index of the analyte has values between 1.33 and 1.36, which is true for most practical cases.

Acknowledgements. The work was supported by the IMT Core Program NanoEl, within the PNCDI 2022–2026, carried out with the support of Romanian Ministry of Research, Innovation and Digitization, project No. 2307 and "MicroNEx", Contract nr. 20 PFE /30.12.2021, financed by the Ministry of Research, Innovation and Digitization through Program 1–Development of the National R & D System, Subprogram 1.2–Institutional Performance–Projects for Institutional Excellence.

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