Waveguide-Based Refractometers Using Bulk, Long-and Short-Range Surface Plasmon Modes: Comparative Study

Anton V. Dyshlyuk ¹⁰, Oleg B. Vitrik, and Uliana A. Eryusheva

Abstract—We present a numerical study comparing three con-5 figurations of the waveguide-based surface plasmon resonance re-6 fractometer: without a buffer layer based on the excitation of the 7 8 bulk surface plasmon mode, and with a buffer layer using the symmetric (long-range) and antisymmetric (short-range) plasmon 9 10 modes. Optimal conditions ensuring the sharpest resonant dip in the refractometer's transmission spectrum are identified. Relative 11 merits of various configurations in terms of the figure-of-merit 12 parameter, local sensitivity to refractive index variations near the 13 metal film, and the size of the sensing element are quantified and 14 15 discussed.

Index Terms—Biosensing, chemosensing, long-range surface
 plasmon mode, short-range surface plasmon mode, SPR, surface
 plasmon resonance, waveguide-based SPR-refractometer.

19

1

2

3

I. INTRODUCTION

EFRACTOMETRIC sensors based on surface plasmon 20 resonance (SPR) represent a topical trend in modern bio-21 and chemosensing technologies [1]–[4]. Sensors of this kind use 22 resonant excitation of surface plasmon waves (coupled oscilla-23 tions of free electron density and electromagnetic field bound to 24 a metal-dielectric interface) to detect minute variations in refrac-25 tive index induced by (bio)chemical reactions near the interface 26 [4]-[6]. 27

The most common configuration of the SPR-refractometer is the well-known Kretschmann scheme, in which surface plasmons are excited by a beam of light incident from within a prism on its metal-coated facet [4]–[6]. This configuration is widely used in laboratory-based biochemical researches, but it is not suited for making portable and inexpensive sensors, including disposable and point-of-care devices. Considerable research

Manuscript received May 30, 2018; revised August 9, 2018; accepted September 2, 2018. The work was supported by the Russian Science Foundation under Grant 16-12-10165. (*Corresponding author: Anton V. Dyshlyuk.*)

A. V. Dyshlyuk is with the Far Eastern Federal University, Vladivostok 690090, Russia, and also with Vladivostok State University of Economics and Service, Vladivostok 690014, Russia (e-mail: anton_dys@mail.ru).

O. B. Vitrik is with the Institute of Automation and Control Processes (Far Eastern Branch of Russian Academy of Sciences), Vladivostok 690041, Russia, and also with the Far Eastern Federal University, Vladivostok 690090, Russia (e-mail: oleg_vitrik@mail.ru).

U. A. Eryusheva is with the Far Eastern Federal University, Vladivostok 690090, Russia (e-mail: eriusheva.ua@students.dvfu.ru).

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/JLT.2018.2871935

efforts, therefore, are devoted to the development of waveguide-35 based SPR-refractometers in which a surface plasmon mode 36 (SPM) is excited by modes of a dielectric waveguide [5]–[14], 37 [18], [19]. Sensors of this type, in contrast to the Kretschmann 38 configuration, can be easily miniaturized and coupled to fiber 39 and integrated optics elements, can be used for measurements 40 in situ and in hard-to-reach locations, as well as aid in cost 41 reduction of SPR bio- and chemosensing systems [7]-[11]. 42

1

Among various types of waveguide-based SPR-refractom-43 eters known to date the simplest one is probably the waveguide 44 analog of the Kretschmann scheme, in which a metal film is de-45 posited directly onto the light-guiding core of a waveguide [5]-46 [8], [10], [14]. Other configurations have also been proposed, 47 which use a buffer layer between the core and the metal film 48 with the refractive index close to that of the ambient medium 49 [8]–[10], [15]–[19]. In the latter case it is possible to make use 50 of either symmetric (long-range) or antisymmetric (short-range) 51 surface plasmon modes arising due to the hybridization of sur-52 face plasmon modes supported by different sides of a thin metal 53 film [5], [6]. 54

We should note that in the SPR-refractometer without a buffer 55 layer, similarly to the Kretschmann scheme, the refractive index 56 of the waveguiding layer is typically much larger than that of 57 the ambient medium. This makes the propagation constants of 58 the surface plasmon modes at two sides of the metal film quite 59 different so that they cannot hybridize effectively even if the 60 film is very thin. Hence, the plasmon mode excited in the SPR-61 refractometer without a buffer layer is localized at the metal 62 ambient medium interface and is very close in its characteristics 63 to the SPM at the surface of a bulk metal. We shall thus refer 64 to it as the 'bulk surface plasmon mode' (BSPM) as opposed to 65 the symmetric surface plasmon mode (SSPM) and antisymmet-66 ric surface plasmon mode (ASPM) in the refractometer with a 67 buffer layer. 68

Symmetric, antisymmetric and bulk plasmon modes differ 69 in their propagation constants, losses, penetration depths and 70 sensitivity to the ambient refractive index [6]. As to which of 71 the modes is most suitable for building an SPR-refractometer 72 there seems to be no apparent consensus in the published litera-73 ture. Those authors who propose refractometers based on SSPM 74 emphasize its lower losses and, correspondingly, a narrower res-75 onant dip in the transmission spectrum as well as higher spectral 76 sensitivity [15]–[17]. 77

0733-8724 © 2018 IEEE. Personal use is permitted, but republication/redistribution requires IEEE permission. See http://www.ieee.org/publications_standards/publications/rights/index.html for more information.



Fig. 1. Schematic representation of the waveguiding structures under study: (a) SPR-refractometer without a buffer layer based on the excitation of bulk surface plasmon mode; (b) SPR-refractometer with buffer layer based on excitation of either symmetric (long-range) or antisymmetric (short-range) surface plasmon modes.

Other authors point out a higher degree of field localization of 78 ASPM, which favors detection of local variations of refractive 79 index in a thin layer near the metal film as well as its very high 80 81 losses aiding in miniaturization of the SPR-sensor [18], [19]. In [6] a detailed comparison of prism-based configurations using 82 BSPM, SSPM and ASPM is made. However, for waveguide-83 based SPR-sensors a direct and quantitative comparison, to the 84 best of our knowledge, has not been carried out. The purpose 85 86 of this paper is thus a comparative analysis of waveguide-based 87 refractometers using bulk, symmetric and antisymmetric surface plasmon modes. 88

89

II. METHODOLOGY

Schematic diagrams showing BSPM- (a), SSPM- and ASPM-90 based (b) refractometers under study are presented in Fig. 1. In 91 all three cases the refractometer is made up of three sections: 92 1, 3 - input and output waveguide sections without metal film, 93 2 - metallized sensing section. The metal film is in contact with 94 95 a liquid ambient medium whose refractive index (n_{ext}) is to be measured. We chose silver as a material of the metal film and 96 took its complex-valued permittivity data from handbook [20]. 97 For SPR to be possible the electric field polarization of guided 98 light is assumed to be in the plane of Fig. 1. 99

The parameters of the waveguiding layer are chosen so as to 100 ensure its single-mode operation. The guided light in Sections 1 101 and 3 is then described by a single TM fundamental mode. To 102 analyze light propagation in the metallized section two different 103 approaches can be employed. Within the first one, the guided 104 105 light is considered to be a superposition of two hybrid modes of the multilayer structure of Section 2 viewed as a whole [21]. In 106 107 the second approach, the metallized section is assumed to support waveguide and surface plasmon modes viewed separately. 108 The interaction between these modes arising when the real parts 109 of their propagation constants are equal or close to one another, 110 as described by the coupled mode theory, leads to the modal 111 112 amplitudes becoming functions of the distance along the wave-113 guide [21]. This second approach is physically more elucidating

and made use of for preliminary analysis and interpretation of 114 numerical results. For numerical modeling, however, it is most 115 convenient to take advantage of the first approach since it is 116 readily available as a standard methodology of modern photon-117 ics simulation software, such as Lumerical Mode Solutions used 118 in this work. 119

To simplify simulation we assumed 2D geometry of the structures under study, which corresponds to an idealized slab waveguide. The obtained results, however, do provide a qualitative understanding of metrological performance of similar 3D structures such as integrated optical refractometers of rectangular cross-section [8], [14], [18], [19] or fiber optic side-polished SPR-probes [7]–[12].

The basic metrological parameter of an SPR-refractometer is 127 its spectral sensitivity [6]: 128

$$S_{RI} = \frac{d\lambda_{SPR}}{dn_{ext}} = \frac{d\lambda_{SPR}}{dn'_{SP}} \cdot \frac{dn'_{SP}}{dn_{ext}} = S_1 S_2, \qquad (1)$$

where λ_{SPR} is the central wavelength of the resonant dip in the 129 refractometer's transmission spectrum, n'_{SP} – the real part of sur-130 face plasmon mode's effective refractive index, $S_1 = \frac{d\lambda_{SPR}}{dn'_{SP}} = 131$ $\frac{1}{\frac{dn_{wg}}{d\lambda}} - \frac{dn'_{SP}}{d\lambda}$ - the instrumental sensitivity which depends on the 132 intersection angle of the dispersion curves of the waveguide and 133 surface plasmon modes, λ – wavelength, n_{wg} – effective index of 134 the waveguide mode, S_2 - the physical sensitivity of the surface 135 plasmon mode's effective index to the ambient refractive index. 136

Apart from spectral sensitivity, SPR-refractometer's resolu- 137 tion is also affected by the width and depth of the resonant dip, 138 noise level in the detection system and other factors [6]. For 139 the sake of comparison of different refractometric configura- 140 tions, however, it suffices to take into account that resolution 141 is inversely proportional to S_{RI} and the contrast of the resonant 142 dip defined as its depth-to-width ratio [6]. Since attenuation of 143 guided light in a waveguide-based SPR-refractometer can reach 144 several orders of magnitude and its transmission is most con- 145 veniently expressed in logarithmic units, it seems reasonable 146 to characterize the width of the dip not by the conventional 147 half-width, but rather by a full width at square root of the min- 148 imum (FWSRM) transmission value which corresponds to the 149 half-width of the dip on a logarithmic scale. This width, as 150 calculations show, is larger for higher SPM losses and smaller 151 intersection angle of the dispersion curves of SPM and the wave- 152 guide mode. 153

The depth of the dip depends primarily on the length of the 154 metallized section L. The best resolution is achieved with the 155 deepest resonant dip, but if its depth exceeds the dynamic range 156 of the spectrum analyzer employed, the shape of the dip can 157 be distorted by noise. With this in mind we choose the length 158 of the sensing section, in all cases, so that the attenuation at 159 resonance is \sim 80 dB, which corresponds roughly to the dynamic 160 range of a modern optical spectrum analyzer (such as Yokogawa 161 AQ6370D).

To compare metrological performance of different refractometric configuration we thus use the so-called Figure-of-Merit 164 (FOM) parameter defined as the ratio of spectral sensitivity to 165 the logarithmic half-width of the resonant dip. Refractometric 166 resolution is inversely proportional to FOM [6] so the best 167



Fig. 2. Spectral dependencies of the effective refractive index (a) and losses (b) of the hybrid modes of the metallized section, as well as the transmission spectrum of the refractometer (c) at th_m = 60 nm, n_{ext} = 1.4, L = 500 μ m. The insets show MMLS profiles at resonance ($\lambda = 0.703 \ \mu$ m, insets 1, 2) and off resonance ($\lambda = 0.64 \ \mu$ m, insets 3, 4).

SPR-refractometer with the minimum resolution is the one withthe largest FOM value.

Another parameter of an SPR-refractometer, which is im-170 171 portant for bio- and chemosensing applications, is the penetration depth (d_{SP}) of the surface plasmon mode into the ambient 172 medium conventionally defined at the 1/e level of the SPM in-173 tensity profile. That is because the thickness of the sensing layer 174 of ligand molecules (d_{lig}) can be much smaller than d_{sp}. In this 175 case an SPR-refractometer is more appropriately characterized 176 by the so-called local sensitivity: $S_{loc} \propto S_{RI} \frac{d_{lig}}{d_{SR}}$, which takes 177 proper account of the sensitivity of SPM's propagation constant 178 to refractive index variations in a thin layer near the metal film 179 [6]. It then follows that refractometric resolution with respect 180 to local RI variations should be proportional to the "local res-181 olution coefficient" (LRC) defined as the ratio of d_{SP} to FOM, 182 which we shall use to compare different SPR-refractometers in 183 terms of local resolution - the smallest LRC value corresponds 184 to the best configuration. 185



III. RESULTS

187 A. SPR-Refractometer Without a Buffer Layer

In practical terms it is advantageous to build an SPR-188 refractometer with the most common and readily available op-189 tical materials, so let us choose SiO₂ ($n_s \sim 1.45$ [20]) as a 190 substrate material and PMMA ($n_w \sim 1.49$ [22]) as a waveguid-191 ing layer material. Numerical calculations then show that for 192 the waveguiding layer thickness th_w = 1.5 μm and ambient re-193 fractive index $n_{ext} = 1.4$ the dispersion curves of the separately 194 considered waveguide and bulk surface plasmon modes inter-195 sect in the near infrared spectral range (Fig. 2a, dotted lines). 196 By the separately considered BSPM we mean the mode of the 197 198 metal film localized at metal ambient medium interface, with 199 the metal film being bounded on one side by the semi-infinite



Fig. 3. Effective index and loss spectra of hybrid MMLS, transmission spectra of the refractometer, and electric field amplitude distribution in the metallized section at the resonant wavelength at $n_{ext} = 1.4$, $L = 500 \,\mu$ m and $th_m = 45 \,\text{nm}$ (a), (b), (c), (d), 68 nm (e), (f), (g), (h), 69 nm (i), (j), (k), (l), 74 nm (m), (n), (o), (p).

ambient medium and, on the other side, by semi-infinite di- 200 electric with refractive index n_w . By the separately considered 201 waveguide mode (WM) we mean the single fundamental mode 202 of the waveguiding layer bounded by semi-infinite substrate and 203 semi-infinite ambient medium. 204

According to the coupled mode theory, near the wavelength 205 of intersection of WM and BSPM dispersion curves pronounced 206 losses can occur in Section 2 as a result of transfer of guided 207 light energy to surface plasmons, provided that the WM-BSPM coupling coefficient is sufficiently large. This is indeed the 209 case for the metal film thickness $th_m = 60 \text{ nm}$, which is con-210 firmed by the results of calculation of the effective index spectra 211 (Fig. 2a, solid lines), loss spectra (Fig. 2b) and profiles (insets 1-212 4) of the hybrid modes of multilayer structure (MMLS) forming 213 Section 2. It is evident from insets 1 and 2 that at the resonant 214 wavelength MMLS, with their profiles made up of the elements 215 of both BSPM and WM, are indeed a result of the hybridization 216 of the latter modes. Since both MMLS have similar profiles at 217 this wavelength and, therefore, similar overlap integrals with the 218 waveguide mode of Section 1, they are excited at the beginning 219 of Section 2 with about the same amplitudes. Their losses are 220 equally high ($\sim 1700 \text{ dB/cm}$) and result in the attenuation of 221 guided light power by \sim 80 dB for the length of the metallized 222 section L = 0.5 mm. Off the resonant wavelength, as seen from 223 Fig. 2b and insets 3-4, both profiles and losses of MMLS are 224 quite different. The low loss mode is closer in its profile to the 225 waveguide mode of Section 1 and is, therefore, excited much 226 more efficiently. As a result, there is no significant attenuation 227 of light in Section 2 at this wavelength. It is in this way that a 228 pronounced dip is formed in the transmission spectrum of the 229 refractometer (Fig. 2c). 230

Numerical calculations show that, depending on the thickness 231 of the metal film, the formation of the resonant dip can occur 232 in two distinct scenarios. If the film thickness is 68 nm or less 233 there is an anticrossing in the effective index spectra of hybrid 234 MMLS, and a crossing in their loss spectra. This is illustrated by 235 Fig. 2a, b ($th_m = 60 \text{ nm}$) and Fig. 3a, b, e, f ($th_m = 45; 68 \text{ nm}$). 236 At film thicknesses of 69 nm or more, on the contrary, the MMLS 237 spectra intersect, while their loss spectra do not (Fig. 3i, j, m, n 238 $(th_m = 69, 74 \text{ nm})).$ 239

These scenarios can be associated with two different coupling 240 regimes between the separately considered WM and BSPM. 241 The first scenario can be regarded as strong coupling whereby a 242 243 periodic power exchange takes place at the resonant wavelength between the coupled modes (see also [23] for discussion and 244 [24] for experimental observation of this). This is illustrated by 245 the distribution of the electric field amplitude in Section 2 at a 246 film thickness of 45 nm (Fig. 3d). From the point of view of 247 the entire multilayer structure forming Section 2, this exchange 248 249 corresponds to interference beats of hybrid MMLS with a period of $\lambda/\Delta n$, where Δn is the difference in their effective indexes at 250 the resonant wavelength. Note that this period increases with 251 increasing film thickness and, for example, at $th_m = 68 \text{ nm}$, 252 it becomes larger than the characteristic attenuation length of 253 guided light in Section 2. In this case, the exchange of power 254 between WM and BSPM proceeds too slowly to be seen against 255 the background of the overall attenuation of light in Section 2 256 (Fig. 3h, $th_m = 68 \text{ nm}$). 257

The second hybridization scenario can be associated with a 258 weak-coupling regime in which such a periodic power exchange 259 260 between the waveguide and surface plasmon modes at the resonant wavelength does not occur (see [24] for experimental ob-261 servation of this regime). In terms of MMLS, this corresponds to 262 a situation where interference beats between them are not pos-263 264 sible due to their propagation constants being equal at $\lambda = \lambda_{SPR}$ (Fig. 3i, m). 265

We must emphasize that the terms "strong" and "weak" coupling are understood here differently than in the context of coupling between lossless modes, and both apply to the resonant wavelength where the real parts of the propagation constants of the coupled modes are exactly equal.

It follows from the coupled mode theory [21] that the coupling 271 regime between WM and BSPM is determined by whether or 272 not the coupling coefficient D is larger than the difference of 273 their effective indexes. At the resonant wavelength the latter 274 reduces, due to WM being lossless, to the imaginary part of 275 the BSPM effective index n''_{SP} . If $D > n''_{SP}$, the dependences 276 of the coupled modes amplitudes on the coordinate along the 277 278 fiber can be shown to be quasiperiodic, which corresponds to the strong-coupling regime, and for $D < n''_{SP}$ they acquire a 279 quasi-exponential character corresponding to the weak coupling 280 regime. 281

The coupling coefficient is defined primarily by the thick-282 ness of the metal film: for larger th_m the profiles of WM and 283 BSPM overlap less effectively which leads to lower D value and, 284 therefore, weaker coupling. If the coupling becomes too weak 285 $(D << n''_{SP})$, say at th_m = 74 nm, the transfer of guided light 286 energy to surface plasmons becomes inefficient which consid-287 erably reduces the depth of the resonant dip (Fig. 30). In terms 288 289 of MMLS it is explained by the fact that their profiles and losses at the resonant wavelength differ, with lower loss MMLS being 290 291 closer in its profile to the fundamental mode of Section 1. It is, as a result, excited more effectively and to a greater extent 292 affects the overall transmission of the structure, which leads to 293 the observed reduction of the depth of the dip. 294

On the other hand, if the coupling is too strong (D >> n''_{SP}), for example, at th_m = 45 nm, the spectral range around λ_{SPR} where the transfer of energy to surface plasmons is effective



Fig. 4. Calculated transmission spectra of the refractometer for $n_{ext}=1.395-1.41, th_m=68\,nm, L=0.5\,mm$. Shown in the insets below are the effective index and loss spectra of MMLS of Section 2 at $n_{ext}=1.395;\,1.401;\,1.406;\,1.41.$

gets wider, which leads to the broadening of the resonant dip 298 (Fig. 3c). We thus conclude that the sharpest resonant dip is 299 obtained with the critical coupling - just at the border between 300 weak and strong coupling regimes. At $n_{ext} = 1.4$ this is achieved 301 with a film thickness of 68 nm (Fig. 3g). 302

The ambient refractive index, however, does not remain con-303 stant in the course of refractometric measurements. Its varia- 304 tion shifts the resonant wavelength, which, for a fixed value 305 of th_m, is inevitably accompanied by changes in the resonant 306 dip contrast. This is illustrated in Fig. 4 depicting transmission 307 spectra of the refractometer calculated for $th_m = 68 \text{ nm}, n_{ext} =$ 308 1.395-1.41, L = 0.5 mm. As evident from the dispersion curves 309 of hybrid MMLS shown in the insets at the bottom of Fig. 4 the 310 coupling between WM and BSPM gets stronger with increas- 311 ing n_{ext} and λ_{SPR} . This is explained by the fact that, firstly, the 312 profiles of WM and BSPM broaden as the wavelength increases 313 and overlap more effectively thus leading to a larger coupling 314 coefficient. Secondly, n''_{SP} value responsible for the losses of 315 BSPM tend to decrease with increasing wavelength [6], which 316 also makes the coupling stronger. 317

Thus the depth of the resonant dip first gradually growths 318 while shifting from left to right with increasing n_{ext} as the cou- 319 pling gets stronger but is still in the weak coupling regime 320 $(n_{ext} < 1.4)$. The switching to the strong coupling regime oc-321 curs at $n_{ext} \sim 1.4$ after which the coupling continues to grow 322 stronger as seen from the growing difference in the effective 323 indexes of MMLS at the resonant wavelength (marked with 324 arrows in the insets of Fig. 4). At $n_{ext} > 1.4$ one can also ob-325 serve slight quasiperiodic variations in the depth of the resonant 326 dip. They arise from the periodic power exchange between the 327 waveguide and surface plasmon modes resulting into the guided 328 light, depending on the period of the exchange, being predom-329 inantly localized at the end of Section 2 either in the region of 330 the waveguiding layer or near the metal film. This affects the 331 transmission loss between Sections 2 and 3, which varies as the 332



Fig. 5. Effective index spectra for the separately considered waveguide and bulk surface plasmon modes as well as transmission spectra of the refractometer at $h_m = 58 \text{ nm}$, $h_w = 1 \mu m$, L = 0.2 nm, $n_{ext} = 1.34-1.37$ (a), (b) and at $h_m = 75 \text{ nm}$, $h_w = 2.5 \mu m$, L = 1.3 mm, $n_{ext} = 1.433-1.439$ (c), (d). The upper-right inset shows the spectral dependences of losses and depth of penetration of BSPM into the ambient medium.

period of the exchange gets shorter with stronger coupling, thusleading to the observed variations in the depth of the dip.

When the ambient refractive index exceeds \sim 1.406 the resonant dip broadens due to WM-BSPM coupling becoming overly strong and its depth decreases due to lower losses of BSPM at longer wavelengths.

It then seems reasonable to define a range of efficient re-339 fractometric measurements (Δn_{ext}) as the range of n_{ext} values 340 341 for which the depth of the resonant dip is less than the maximum depth by not more than an arbitrary threshold value, say 342 20 dB. For the configuration under study, as seen from Fig. 4, 343 this corresponds roughly to next ranging from 1.395 to 1.41, 344 i.e., $\Delta n_{ext} \cong 0.015$. It also follows from the analysis of the 345 transmission spectra in Fig. 4 that the spectral sensitivity of 346 the refractometer is $S_{RI} \cong 6800 \text{ nm/ RI}$ unit (RIU), logarith-347 mic half-width of the dip in the middle of the measured next 348 range – FWSRM \cong 25 nm. The penetration depth of BSPM into 349 the ambient medium at $\lambda \sim 700$ nm is $d_{sp} \cong 120$ nm (see the 350 inset of Fig. 5), which yields FOM \cong 270 and LRC \cong 0.44. 351

It should be noted that the SPR-refractometer under con-352 sideration can be used for measuring other values of ambient 353 refractive index, both higher and lower than 1.4. For example, 354 at $n_{ext} \sim 1.35$ the phase-matching condition between the wave-355 guide and surface plasmon modes is fulfilled near $\lambda = 550$ nm 356 (Fig. 5a). The optimal film thickness in this case is 58 nm. For 357 the waveguide layer to remain in the single-mode regime its 358 width is reduced to 1 micron. Since the losses of BSPM in this 359 spectral range are several times higher than those at $\lambda \sim 700$ nm 360 (inset of Fig. 5) we also reduce the length of the metallized 361 section to 0.2 mm. 362

In spite of the higher losses of BSPM the width of the resonant dip turns out in this case to be less than in the previous one: FWSRM \cong 16 nm (at n_{ext} \cong 1.35), which can be explained by a much larger angle of intersection of WM and BSPM dispersion curves (Fig. 5a). It is for the same reason that, although physical sensitivity of BSPM's effective index to the ambient RI is larger at shorter wavelengths [6], the overall spectral sensitivity turns out in this case to be about 2.5 times lower 370 than that at $\lambda \sim 700$ nm: S_{RI} $\cong 2600$ nm/RIU due to a drop 371 in the instrumental sensitivity. The rage of measured refractive 372 index is correspondingly larger: $\Delta n_{ext} \cong 0.03$. FOM amounts 373 to ~ 162 which is more than 1.5 times worse than in the previous 374 case. The penetration depth of BSPM into the ambient medium, 375 however, at $\lambda \sim 550$ nm is only ~ 70 nm (inset of Fig. 5), so 376 in terms of the local resolution there is virtually no difference 377 from the previous case: LRC ≈ 0.43 . 378

At a higher value of the ambient refractive index: $n_{ext} \sim 1.435$ 379 the phase-matching condition between the waveguide and sur-380 face plasmon modes is fulfilled at $\lambda \sim 1000$ nm (Fig. 5c). The 381 optimal waveguide width and metal film thickness in this case 382 are 2.5 μ m and 75 nm, respectively. The losses of BSPM in this 383 spectral range are much lower than at $\lambda \sim 700$ nm or $\lambda \sim 550$ nm, 384 so to get a $\sim 80 \text{ dB}$ resonant dip the length of the metallized sec-385 tion has to be extended to L = 1.3 mm. Secondly, the dispersion 386 curves of WM and BSPM intersect here at a much smaller an-387 gle than in both cases considered above. This leads to a much 388 higher spectral sensitivity due to a larger instrumental contri-389 bution: $S_{RI} \cong 26000 \text{ nm/ RIU}$, narrowing of the measured RI 390 range: $\Delta n_{ext} \cong 0,008$, and broadening of the resonant dip. The 391 latter feature is, however, partially compensated by the lower 392 losses of BSPM in this spectral range resulting in FWSRM \cong 393 44 nm (at $n_{ext} \approx 1.435$). There is thus a significant advantage 394 in terms combination of spectral sensitivity and width of the dip 395 as compared to the previous cases: FOM \cong 590. The local reso-396 lution is, however, virtually unchanged because of much deeper 397 penetration of BSPM into the ambient medium at $\lambda \sim 1000$ nm 398 $(d_{SP} \cong 270 \text{ nm}, \text{ inset of Fig. 5})$: LRC $\cong 0.46$. 399

B. SPR-Refractometer Based on Symmetric (Long-Range)400Surface Plasmon Mode401

Introduction of a buffer layer between the waveguide and 402 metal film with the refractive index close to that of the am-403 bient medium enables one to build an SPR-refractometer both 404 on symmetric (long-range) and antisymmetric (short-range) sur-405 face plasmon modes [6]. SSPM and ASPM differ significantly in 406 their properties both from each other and from the bulk surface 407 plasmon mode considered above. The metrological parameters 408 of corresponding SPR-refractometers can, therefore, be widely 409 different as well. To gain a benefit in metrological performance 410 one must to the fullest possible extent exploit the advantages 411 that a particular plasmon mode has to offer in terms of building 412 an SPR-refractometer. 413

As for the long-range surface plasmon mode its major strength 414 is in its low propagation losses [6], [15]–[17]. This enables one 415 to obtain a reasonably narrow resonant dip even with a very 416 small intersection angle between WM and SSPM dispersion 417 curves, which may yield a very high spectral sensitivity due 418 to a large instrumental contribution. The losses of SSPM tend 419 to decrease for larger wavelength and thinner metal film [6], 420 which makes it reasonable to use a long-wavelength spectral 421 range and a thin metal film. Making the film too thin, how-422 ever, is not practical and can be technologically challenging. 423 At too long a wavelength, on the other hand, the intersection 424 angle can become too small to produce a distinct resonant dip 425



Fig. 6. Dispersion curves of the separately considered waveguide and symmetric surface plasmon modes (a) and transmission spectra of the SSPM-based refractometer (d) for $n_{ext} = 1.3299-1.3302$; effective index and loss spectra of the hybrid MMLS of the metallized section for $n_{ext} = 1.3299$ (b), (e) and 1.33 (c), (f) (L = 60 mm, th_w = 200 nm, th_b = 13.3 μ m, th_m = 20 nm).

in spite of SSPM's low losses. With thus choose as a com-426 promise th_m = 20 nm and $\lambda \sim 1000$ nm. We note also that the 427 effective index of the long-range surface plasmon mode is much 428 lower than those of ASPM and BSPM, so to phase-match it to 429 430 the waveguide mode one has to use materials with low optical density. The specified requirements are fulfilled e.g., with the 431 following waveguiding structure: substrate made of Cytop poly-432 mer ($n_s \sim 1.34$ [25]), waveguiding layer – MgF₂ ($n_w \sim 1.37$ [26], 433 434 $th_w = 200 \text{ nm}$), buffer layer – Cytop, silver film ($th_m = 20 \text{ nm}$).

Fig. 6a shows the dispersion curves of the separately con-435 sidered WM and SSPM calculated for the chosen structure at 436 $n_{ext} = 1.33$. As seen from the figure the phase-matching be-437 tween the two modes can be achieved near $\lambda = 1040$ nm. To 438 ensure the maximum contrast of the resonant dip we also re-439 quire the switching from the weak to strong regime of WM-440 SSPM coupling to occur around this wavelength. Unlike the 441 previously considered configuration, in the SPR-refractometer 442 with a buffer layer it is the thickness of the buffer layer that is 443 primarily responsible for the coupling regime. Calculation show 444 that the optimal value of th_b at which the switching of coupling 445 regimes occurs near $\lambda = 1040$ at $n_{ext} \approx 1.33$ amounts to 13.3 446 microns (Fig. 6b, c, e, f). 447

The transmission spectra of the refractometer calculated 448 for $n_{ext} = 1.3299 - 1.3302$, th_b = 13.3 μ m are shown in Fig. 6d. 449 One can conclude from the figure that spectral sensitiv-450 ity in this case amounts to as high as ~ 120000 nm/RIU, 451 $\Delta n_{ext} \cong 0,0004$, FWSRM $\cong 18$ nm (at $n_{ext} \cong 1.3301$), i.e., 452 FOM \cong 6670, which is more than an order of magnitude 453 higher than that of the SPR-refractometer without a buffer 454 layer. In spite of the penetration depth of SSPM into the 455 ambient medium being much higher than that of BSPM 456 $(d_{SP} \cong 580 \text{ nm at } \lambda \sim 1050 \text{ nm})$ in terms of local resolution 457 the SPR-refractometer based on SSPM has a significant advan-458 tage as well: LRC \cong 0.09 which is ~5 times below that of 459 SPR-refractometer without a buffer layer. We must note, how-460 ever, that the advantage in metrological performance arises from 461 the low losses of SSPM (~30 dB/cm at $\lambda \sim 1050$ nm) and it 462 comes, therefore, at a cost of extending the length of the sensing 463 section: an \sim 80dB resonant dip is achieved with the sensing 464 section being as long as 6 cm. 465

If needed the sensing section can be shortened by choosing the parameters of the structure so that the SPR condition is fulfilled at a shorter wavelength where SSPM has higher losses. 468 For example, at $th_w = 400 \text{ nm}$ and $n_{ext} = 1.33$ the waveguide 469 mode is phase-matched to SSPM at around $\lambda = 600$ nm. The 470 optimal thickness of the buffer layer is $th_b = 2.6 \,\mu m$. The 471 losses of SSPM in this spectral range are about an order of 472 magnitude higher than those at $\lambda \sim 1000$ nm: ~ 310 dB/cm 473 enabling 10-fold shortening of the sensing section: L = 6 mm. 474 The spectral sensitivity, however, turns out in this case to be 475 only about a tenth of that at $\lambda \sim 1000$ nm due to a sharp 476 drop in the instrumental contribution: $S_{RI} \cong 16000 \text{ nm/ RIU}, 477$ which is accompanied by broadening of the RI measurement 478 range: $\Delta n_{ext} \cong 0.003$ and some narrowing of the resonant dip: 479 FWSRM \cong 12 nm. Thus, in terms of combination of sensitivity 480 and resonant dip width such a configuration is more than 5 times 481 inferior to the previous one: FOM \cong 1330. The local resolution 482 is, however, not much worse than that in the previous case due 483 to much a lower penetration depth of SSPM at $\lambda \sim 600$ nm 484 than at $\lambda \sim 1000$ nm (d_{sp} $\cong 200$ nm): LRC $\cong 0.15$. 485

C. SPR-Refractometer Based on the Antisymmetric 486 (Short-Range) Surface Plasmon Mode 487

From the analysis of the properties of the antisymmetric sur- 488 face plasmon mode [6] one can conclude that its main advan- 489 tages in terms of building an SPR refractometer are as follows. 490 Firstly, it has a higher degree of field localization near the film 491 which may lead to better sensitivity to local variations of refrac- 492 tive index. Secondly, it has a higher physical sensitivity to the 493 ambient refractive index as compared to SSPM. Thirdly, higher 494 losses of ASPM allow one to obtain a deep resonant dip with a 495 very short sensing section, which aids in miniaturization of the 496 refractometer. All of these features become more pronounced 497 with decreasing wavelength and metal film thickness [6]. An-498 other circumstance to take into account is that, as calculations 499 show, when the media on two sides of the film differ in refrac- 500 tive indexes the profile of ASPM tends to shift to the optically 501 denser medium, which brings about additional increase in sen- 502 sitivity to the refractive index of that medium. Thus in order to 503 exploit ASPM's advantages to the fullest degree one should use 504 shorter wavelength range, very thin film and make the refractive 505 index of the buffer layer somewhat lower than that of the am- 506 bient medium. Due to the effective index of ASPM being quite 507 high [6], to enable its phase-matching with the waveguide mode 508 one should use for the waveguiding layer a high optical density 509 material. 510

The stated requirements are satisfied e.g., with the following 511 structure: substrate – SiO₂, waveguiding layer – Si₃N₄ ($n_w \sim 2$ 512 [27], th_w = 250 nm), buffer layer – Teflon AF2400 ($n_b \sim 1.28$ 513 [28]), silver film (th_m = 20 nm), ambient medium ($n_{ext} > n_b$). 514

Fig. 7a shows the dispersion curves of the separately 515 considered waveguide and antisymmetric plasmon modes 516 calculated for the chosen structure at different n_{ext} values in 517 the range 1.34–1.37. As one can see, the SPR condition is 518 fulfilled at $\lambda \sim 640$ nm where ASPM losses are found to be 519 as high as ~42000 dB/cm. The optimal thickness of the buffer 520 layer at which the switching of WM-ASPM coupling regimes 521 occurs near this wavelength is th_b = 180 nm (Fig. 7b, c, e, f). 522 The losses of hybrid MMLS at the resonant wavelength reach 523

	SPR-refractometer without a buffer layer			SPR-refractometer based on long- range surface plasmon mode		SPR-refractometer based on short- range surface plasmon mode	
Measured RI, $\overline{n_{ext}} \pm \frac{\Delta n_{ext}}{2}$	1.355±0.015	1.404±0.0075	1.437±0.004	1.33±0.0015	1.3301±0.0002	1.355±0.015	1.33±0.01
Resonant wavelength range, nm	530-610	680-780	920-1120	600-650	1030-1080	625-655	900-980
Instrumental sensitivity, S1	2 000	6 000	24 000	34 000	316 000	825	4 350
Physical sensitivity, S ₂	1.26	1.14	1.08	0.47	0.38	1.09	0.85
Spectral sensitivity S _{RI} , nm/RIU	2 600	6 800	26 000	16 000	120 000	900	3 700
FWSRM, nm	16	25	44	12	18	35	65
FOM	162	270	590	1 330	6 670	25,7	57
SPM losses near λ_{SPR} , dB/cm	11 620	3 650	970	310	30	42 000	11 000
Length of the sensing section, mm	0.2	0.5	1.3	6	60	0.04	0.18
SPM penetration, d _{SP} , nm	70	120	270	200	580	44	117
Local resolution coefficient, LRC	0.43	0.44	0.46	0.15	0.09	1.7	2.05

 TABLE I

 Specifications of the SPR-Refractometers Under Study



Fig. 7. Dispersion curves of the separately considered waveguide and antisymmetric surface plasmon modes (a), as well as transmission spectra of the ASPM-based refractometer (d) calculated for $n_{ext} = 1.34-1.37$; effective index and loss spectra of hybrid MMLS of the metallized section calculated for $n_{ext} = 1.37$ (b), (e) and 1.35 (c), (f) (L = 0.04 mm, th_w = 250 nm, th_b = 180 nm, th_m = 20 nm).

524 ~22 000 dB/cm which makes it possible to reduce the length 525 of the sensing section to just $L = 40 \ \mu m$.

The transmission spectra of the refractometer are shown 526 in Fig. 7d. It can be concluded from the figure that the 527 spectral sensitivity is in this case \sim 900 nm/RIU, $\Delta n_{ext} \cong$ 528 0.03, FWSRM \cong 35 nm (at n_{ext} \cong 1.36), and FOM \cong 25.7, 529 which is about an order of magnitude lower than the FOM of the 530 refractometer without a buffer layer and 260 times lower than 531 the FOM of the refractometer on SSPM. The penetration depth 532 of ASPM into the ambient medium, however, at $\lambda \sim 640$ nm is 533 just \sim 44 nm and LRC amounts, therefore, to \sim 1.7. 534

We note that such a low sensitivity results from an extraordi-535 narily low instrumental contribution due to a very large intersec-536 tion angle of WM and ASPM dispersion curves. The parameters 537 of the waveguiding structure can be adjusted to shift the reso-538 nance to a longer wavelength thus decreasing the intersection an-539 gle and enhancing the sensitivity. This will also broaden the res-540 onant dip but due to ASPM losses falling with wavelength some 541 benefit should be expected in terms of FOM parameter (at the ex-542 pense of a longer sensing section). For example, at $th_b = 150 \text{ nm}$ 543 and $n_{ext} \sim 1.33$ the SPR condition is fulfilled at $\lambda \sim 900 \text{ nm}$ 544 where the losses of ASPM amount to ~ 11000 dB/cm. At 545 546 the optimal film thickness $(th_b = 568 \text{ nm})$ an 80-dB resonant dip can be obtained with a sensing section of 180 μ m. 547 The spectral sensitivity is then found to be ~3700 nm/RIU, 548 $\Delta n_{ext} \cong 0.02$, FWSRM $\cong 65$ nm, $d_{SP} \cong 117$ nm, which results in FOM $\cong 57$ and LRC $\cong 2.05$. 550

IV. DISCUSSION 551

The specifications of the studied BSPM, SSPM- and ASPMbased refractometers are summarized in Table I. As seen from the table the difference in metrological performance of different configurations results mainly from their spectral sensitivity. The physical sensitivity, however, does not change much and the observed variations are primarily due to the greatly varying instrumental contribution.

The best specifications are achieved with the SPR-559 refractometer based on symmetric or long-range surface plas-560 mon mode: due to its low losses a sharp resonant dip can be 561 obtained even with a very small intersection angle of WM and 562 SSPM dispersion curves yielding an extremely high instrumen-563 tal and hence overall spectral sensitivity. The advantage in terms 564 of FOM parameter reaches about two orders of magnitude as 565 compared to the ASPM-based SPR-refractometer and one order 566 of magnitude as compared to the SPR-refractometer without a 567 buffer layer. 568

Apart from its low losses the symmetric surface plasmon 569 mode has a larger penetration depth into the ambient medium. 570 In terms of local resolution, therefore, the advantage of using 571 SSPM instead of ASPM or BSPM is less pronounced: LRC is 572 about 20 times lower than that for ASPM and ~6 times lower 573 than that for BSPM. 574

We should also emphasize that the advantage in metrological 575 performance of the SPR-refractometer based on symmetric surface plasmon mode comes at a cost of extending the length of the 577 metallized section: to obtain a resonant dip of the same depth as 578 in ASPM- and BSPM-based refractometers a much longer (up 579 to three orders of magnitude) sensing section is required. 580

The most compact sensing element with the minimum length 581 of the sensing section is characteristic of the SPR-refractometer 582 based on the antisymmetric surface plasmon mode. It has, 583

however, the worst metrological performance among all the 584 studied configurations due to the enormous losses of ASPM. 585

The SPR-refractometer without a buffer layer occupies an 586 587 intermediate position between those based on SSPM and ASPM, both in terms of metrological performance and sensing section 588 length. It has, however, an important practical advantage of 589 having the simplest structure, which facilitates the fabrication 590 process. 591

One can also conclude from the table that the values of 592 593 measured refractive index depend both on the parameters of the metallized section and on the working spectral range. By 594 choosing a longer wavelength range where a surface plasmon 595 mode has lower losses (and using a longer sensing section) one 596 can obtain higher metrological performance in terms of FOM 597 parameter. The local resolution coefficient, however, does not 598 change much since the increase in FOM is offset by a higher 599 penetration depth of SPM into the ambient medium. We also 600 note that if the resonant wavelength is shifted too far into the 601 infrared ($\lambda_{\text{SPR}} \gtrsim 1200 \text{ nm}$) the intersection angle between WM 602 and SPM dispersion curves may get so small that refractometric 603 measurements, in spite of a very high sensitivity, become no 604 longer possible due to smearing out of the resonant dip. 605

606 In closing, we emphasize that metrological parameters summarized in Table I have been obtained in the 2D-geometry 607 608 approximation and depend on the specific choices of materials and geometric parameters of the refractometers. Their pri-609 mary purpose is, therefore, not to characterize performance of 610 practical SPR-sensors but to illustrate in a quantitative manner 611 the relative merits of refractometers based on bulk, symmet-612 ric and antisymmetric surface plasmon modes. The revealed 613 614 patterns and relationships, we believe, are also valid in 3D geometry and do not depend on the specific details of the 615 refractometers. 616

617

V. CONCLUSIONS

We have thus studied three SPR-refractometer configurations: 618 without a buffer layer based on the excitation of the bulk sur-619 face plasmon mode, and with a buffer layer using symmetric 620 (long-range) and antisymmetric (short-range) surface plasmon 621 622 modes. It is shown the highest metrological performance is achieved with the symmetric SPM, which, however, requires a 623 much longer sensing section. If miniaturization of the sensor is 624 of utmost importance the preferred type of plasmon mode to 625 use is the antisymmetric one, which enables minimization of 626 627 the sensing section length at a cost of impaired metrological specifications. Finally, in terms of ease of fabrication the most 628 attractive configuration is that without a buffer layer, which is 629 630 intermediate between SSPM- and ASPM-based refractometers both in terms of metrological performance and sensing section 631 632 length.

633

REFERENCES

- [1] A. Rasooly and K. E. Herold, Biosensors and Biodetection. New York, 634 635 NY, USA: Humana, 2009.
- [2] Ligler F. S. and C. R. Taitt, Optical Biosensors: Today and Tomorrow. 636 637 Amsterdam, The Netherlands: Elsevier, 2011.

- Science & Business Media, 2006, vol. 224. X. Guo and J. Biophoton,"Surface plasmon resonance based biosensor 640 technique: A review," J. Biophoton., vol. 5, pp. 483-501, 2012. 641
- [5] J. Homola, "Surface plasmon resonance sensors for detection of chemical 642 and biological species," Chem. Rev., vol. 108, no. 2, pp. 462-493, 2008. 643
- [6] J. Homola, Surface Plasmon Resonance Based Sensors. Berlin, Germany: 644 Springer-Verlag, 2006. 645
- B. D. Gupta and R. K. Verma "Surface plasmon resonance-based fiber [7] 646 optic sensors: Principle, probe designs, and some applications," J. Sensors, 647 vol. 2009, 2009, Art. no. 979761. 648
- [8] R. Kashyap and G. Nemova, "Surface plasmon resonance-based fiber and 649 planar waveguide sensors," J. Sensors, vol. 2009, 2009, Art. no. 645162. 650
- C. Caucheteur, T. Guo, and J. Albert "Review of plasmonic fiber optic [9] 651 biochemical sensors: Improving the limit of detection," Analytical Bioan-652 alytical Chem., vol. 407, no. 14, pp. 3883-3897, 2015. 653
- [10] E. Klantsataya et al., "Plasmonic fiber optic refractometric sensors: From 654 conventional architectures to recent design trends," Sensors, vol. 17, no. 1, 655 2016, Art. no. 12. 656
- [11] S. K. Srivastava and B. D. Gupta, "Fiber optic plasmonic sensors: Past, 657 present and future," Open Optics J., vol. 7, no. 1, pp. 58-83, 2013. 658
- [12] M. E. Bosch et al., "Recent development in optical fiber biosensors," 659 Sensors, vol. 7, no. 6, pp. 797-859, 2007. 660
- [13] A. V. Dyshlyuk et al., "Numerical and experimental investigation of 661 surface plasmon resonance excitation using whispering gallery modes in 662 bent metal-clad single-mode optical fiber," J. Lightw. Technol., vol. 35, 663 no. 24, pp. 5425-5431, Dec. 2017. 664
- [14] Y.-S. Chu et al., "Surface plasmon resonance sensors using silica-on-665 silicon optical waveguides," Microw. Opt. Technol. Lett., vol. 48, no. 5, 666 pp. 955-957, 2006. 667
- [15] G. G. Nenninger et al., "Long-range surface plasmons for high-resolution 668 surface plasmon resonance sensors," Sensors Actuators B: Chem., vol. 74, 669 no. 1-3, pp. 145-151, 2001. 670
- R. Slavík and J. Homola, "Ultrahigh resolution long range surface [16] 671 672 plasmon-based sensor," Sensors Actuators B: Chem., vol. 123, no. 1, pp. 10-12, 2007. 673
- [17] J. Dostálek, A. Kasry, and W. Knoll, "Long range surface plasmons for 674 observation of biomolecular binding events at metallic surfaces," Plas-675 monics, vol. 2, no. 3, pp. 97-106, 2007. 676
- [18] B. Fan, F. Liu, Y. Li, Y. Huang, Y. Miura, and D. Ohnishi, "Refractive 677 index sensor based on hybrid coupler with short-range surface plasmon 678 polariton and dielectric waveguide," Appl. Phys. Lett., vol. 100, no. 11, 679 2012, Art. no. 111108. 680
- [19] B. Fan et al., "Integrated refractive index sensor based on hybrid coupler 681 with short range surface plasmon polariton and dielectric waveguide," 682 Sensors Actuators B: Chem., vol. 186, pp. 495-505, 2013. 683
- [20] E. D. Palik Handbook of Optical Constants of Solids. New York, NY, 684 USA: Academic, 1998. 685
- A. W. Snyder and J. Love Optical Waveguide Theory. Berlin, Germany: [21] 686 Springer Science & Business Media, 2012. 687
- [22] N. Sultanova, S. Kasarova, and I. Nikolov, "Dispersion properties of opti-688 cal polymers," Acta Physica Polonica-Series A Gen. Phys., vol. 116, no. 4, 689 pp. 585-587, 2009. 690
- M. L. Nesterov, A. V. Kats, and S. K. Turitsyn, "Extremely short-length [23] 691 surface plasmon resonance devices," Optics Express vol. 16, no. 25, 692 pp. 20227-20240, 2008. 693
- [24] H. Ditlbacher et al., "Coupling dielectric waveguide modes to surface 694 plasmon polaritons," Opt. Express, vol. 16, no. 14, pp. 10455-10464, 695 2008 696
- [25] 2018. [Online]. Available: http://www.bellexinternational.com/products/ 697 cvtop/pdf/cvtop-catalog.pdf 698
- [26] H. H. Li, "Refractive index of alkaline earth halides and its wavelength 699 and temperature derivatives," J. Phys. Chem. Ref. Data, vol. 9, no. 1, 700 pp. 161-290, 1980. 701
- [27] H. R. Philipp, "Optical properties of silicon nitride," J. Electrochemical 702 Soc., vol. 120, no. 2, pp. 295-300, 1973. 703
- M. K. Yang, R. H. French, and E. W. Tokarsky, "Optical properties 704 of Teflon AF amorphous fluoropolymers," J. Micro/Nanolithography, 705 MEMS, MOEMS, vol. 7, no. 3, 2008, Art. no. 033010. 706

639

Waveguide-Based Refractometers Using Bulk, Long-and Short-Range Surface Plasmon Modes: Comparative Study

Anton V. Dyshlyuk , Oleg B. Vitrik, and Uliana A. Eryusheva

Abstract—We present a numerical study comparing three con-5 figurations of the waveguide-based surface plasmon resonance re-6 fractometer: without a buffer layer based on the excitation of the 7 8 bulk surface plasmon mode, and with a buffer layer using the symmetric (long-range) and antisymmetric (short-range) plasmon 9 10 modes. Optimal conditions ensuring the sharpest resonant dip in the refractometer's transmission spectrum are identified. Relative 11 merits of various configurations in terms of the figure-of-merit 12 parameter, local sensitivity to refractive index variations near the 13 metal film, and the size of the sensing element are quantified and 14 15 discussed.

Index Terms—Biosensing, chemosensing, long-range surface
 plasmon mode, short-range surface plasmon mode, SPR, surface
 plasmon resonance, waveguide-based SPR-refractometer.

19

1

2

3

I. INTRODUCTION

EFRACTOMETRIC sensors based on surface plasmon 20 resonance (SPR) represent a topical trend in modern bio-21 and chemosensing technologies [1]-[4]. Sensors of this kind use 22 resonant excitation of surface plasmon waves (coupled oscilla-23 tions of free electron density and electromagnetic field bound to 24 a metal-dielectric interface) to detect minute variations in refrac-25 tive index induced by (bio)chemical reactions near the interface 26 [4]-[6]. 27

The most common configuration of the SPR-refractometer is the well-known Kretschmann scheme, in which surface plasmons are excited by a beam of light incident from within a prism on its metal-coated facet [4]–[6]. This configuration is widely used in laboratory-based biochemical researches, but it is not suited for making portable and inexpensive sensors, including disposable and point-of-care devices. Considerable research

Manuscript received May 30, 2018; revised August 9, 2018; accepted September 2, 2018. The work was supported by the Russian Science Foundation under Grant 16-12-10165. (*Corresponding author: Anton V. Dyshlyuk.*)

A. V. Dyshlyuk is with the Far Eastern Federal University, Vladivostok 690090, Russia, and also with Vladivostok State University of Economics and Service, Vladivostok 690014, Russia (e-mail: anton_dys@mail.ru).

O. B. Vitrik is with the Institute of Automation and Control Processes (Far Eastern Branch of Russian Academy of Sciences), Vladivostok 690041, Russia, and also with the Far Eastern Federal University, Vladivostok 690090, Russia (e-mail: oleg_vitrik@mail.ru).

U. A. Eryusheva is with the Far Eastern Federal University, Vladivostok 690090, Russia (e-mail: eriusheva.ua@students.dvfu.ru).

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/JLT.2018.2871935

efforts, therefore, are devoted to the development of waveguide-35 based SPR-refractometers in which a surface plasmon mode 36 (SPM) is excited by modes of a dielectric waveguide [5]–[14], 37 [18], [19]. Sensors of this type, in contrast to the Kretschmann 38 configuration, can be easily miniaturized and coupled to fiber 39 and integrated optics elements, can be used for measurements 40 in situ and in hard-to-reach locations, as well as aid in cost 41 reduction of SPR bio- and chemosensing systems [7]-[11]. 42

1

Among various types of waveguide-based SPR-refractom-43 eters known to date the simplest one is probably the waveguide 44 analog of the Kretschmann scheme, in which a metal film is de-45 posited directly onto the light-guiding core of a waveguide [5]-46 [8], [10], [14]. Other configurations have also been proposed, 47 which use a buffer layer between the core and the metal film 48 with the refractive index close to that of the ambient medium 49 [8]–[10], [15]–[19]. In the latter case it is possible to make use 50 of either symmetric (long-range) or antisymmetric (short-range) 51 surface plasmon modes arising due to the hybridization of sur-52 face plasmon modes supported by different sides of a thin metal 53 film [5], [6]. 54

We should note that in the SPR-refractometer without a buffer 55 layer, similarly to the Kretschmann scheme, the refractive index 56 of the waveguiding layer is typically much larger than that of 57 the ambient medium. This makes the propagation constants of 58 the surface plasmon modes at two sides of the metal film quite 59 different so that they cannot hybridize effectively even if the 60 film is very thin. Hence, the plasmon mode excited in the SPR-61 refractometer without a buffer layer is localized at the metal 62 ambient medium interface and is very close in its characteristics 63 to the SPM at the surface of a bulk metal. We shall thus refer 64 to it as the 'bulk surface plasmon mode' (BSPM) as opposed to 65 the symmetric surface plasmon mode (SSPM) and antisymmet-66 ric surface plasmon mode (ASPM) in the refractometer with a 67 buffer layer. 68

Symmetric, antisymmetric and bulk plasmon modes differ 69 in their propagation constants, losses, penetration depths and 70 sensitivity to the ambient refractive index [6]. As to which of 71 the modes is most suitable for building an SPR-refractometer 72 there seems to be no apparent consensus in the published litera-73 ture. Those authors who propose refractometers based on SSPM 74 emphasize its lower losses and, correspondingly, a narrower res-75 onant dip in the transmission spectrum as well as higher spectral 76 sensitivity [15]–[17]. 77

0733-8724 © 2018 IEEE. Personal use is permitted, but republication/redistribution requires IEEE permission. See http://www.ieee.org/publications_standards/publications/rights/index.html for more information.



Fig. 1. Schematic representation of the waveguiding structures under study: (a) SPR-refractometer without a buffer layer based on the excitation of bulk surface plasmon mode; (b) SPR-refractometer with buffer layer based on excitation of either symmetric (long-range) or antisymmetric (short-range) surface plasmon modes.

Other authors point out a higher degree of field localization of 78 ASPM, which favors detection of local variations of refractive 79 index in a thin layer near the metal film as well as its very high 80 81 losses aiding in miniaturization of the SPR-sensor [18], [19]. In [6] a detailed comparison of prism-based configurations using 82 BSPM, SSPM and ASPM is made. However, for waveguide-83 based SPR-sensors a direct and quantitative comparison, to the 84 best of our knowledge, has not been carried out. The purpose 85 of this paper is thus a comparative analysis of waveguide-based 86 87 refractometers using bulk, symmetric and antisymmetric surface plasmon modes. 88

89

II. METHODOLOGY

Schematic diagrams showing BSPM- (a), SSPM- and ASPM-90 based (b) refractometers under study are presented in Fig. 1. In 91 all three cases the refractometer is made up of three sections: 92 1, 3 - input and output waveguide sections without metal film, 93 2 - metallized sensing section. The metal film is in contact with 94 95 a liquid ambient medium whose refractive index (n_{ext}) is to be measured. We chose silver as a material of the metal film and 96 took its complex-valued permittivity data from handbook [20]. 97 For SPR to be possible the electric field polarization of guided 98 light is assumed to be in the plane of Fig. 1. 99

The parameters of the waveguiding layer are chosen so as to 100 ensure its single-mode operation. The guided light in Sections 1 101 and 3 is then described by a single TM fundamental mode. To 102 analyze light propagation in the metallized section two different 103 approaches can be employed. Within the first one, the guided 104 light is considered to be a superposition of two hybrid modes of 105 the multilayer structure of Section 2 viewed as a whole [21]. In 106 107 the second approach, the metallized section is assumed to support waveguide and surface plasmon modes viewed separately. 108 The interaction between these modes arising when the real parts 109 of their propagation constants are equal or close to one another, 110 as described by the coupled mode theory, leads to the modal 111 112 amplitudes becoming functions of the distance along the wave-113 guide [21]. This second approach is physically more elucidating

and made use of for preliminary analysis and interpretation of 114 numerical results. For numerical modeling, however, it is most 115 convenient to take advantage of the first approach since it is 116 readily available as a standard methodology of modern photon-117 ics simulation software, such as Lumerical Mode Solutions used 118 in this work. 119

To simplify simulation we assumed 2D geometry of the structures under study, which corresponds to an idealized slab waveguide. The obtained results, however, do provide a qualitative understanding of metrological performance of similar 3D structures such as integrated optical refractometers of rectangular cross-section [8], [14], [18], [19] or fiber optic side-polished SPR-probes [7]–[12].

The basic metrological parameter of an SPR-refractometer is 127 its spectral sensitivity [6]: 128

$$S_{RI} = \frac{d\lambda_{SPR}}{dn_{ext}} = \frac{d\lambda_{SPR}}{dn'_{SP}} \cdot \frac{dn'_{SP}}{dn_{ext}} = S_1 S_2, \qquad (1)$$

where λ_{SPR} is the central wavelength of the resonant dip in the 129 refractometer's transmission spectrum, n'_{SP} – the real part of sur-130 face plasmon mode's effective refractive index, $S_1 = \frac{d\lambda_{SPR}}{dn'_{SP}} = 131$ $\frac{1}{\frac{dn_{wg}}{d\lambda}} - \frac{dn'_{SP}}{d\lambda}$ - the instrumental sensitivity which depends on the 132 intersection angle of the dispersion curves of the waveguide and 133 surface plasmon modes, λ – wavelength, n_{wg} – effective index of 134 the waveguide mode, S_2 - the physical sensitivity of the surface 135 plasmon mode's effective index to the ambient refractive index. 136

Apart from spectral sensitivity, SPR-refractometer's resolu- 137 tion is also affected by the width and depth of the resonant dip, 138 noise level in the detection system and other factors [6]. For 139 the sake of comparison of different refractometric configura- 140 tions, however, it suffices to take into account that resolution 141 is inversely proportional to S_{RI} and the contrast of the resonant 142 dip defined as its depth-to-width ratio [6]. Since attenuation of 143 guided light in a waveguide-based SPR-refractometer can reach 144 several orders of magnitude and its transmission is most con- 145 veniently expressed in logarithmic units, it seems reasonable 146 to characterize the width of the dip not by the conventional 147 half-width, but rather by a full width at square root of the min- 148 imum (FWSRM) transmission value which corresponds to the 149 half-width of the dip on a logarithmic scale. This width, as 150 calculations show, is larger for higher SPM losses and smaller 151 intersection angle of the dispersion curves of SPM and the wave- 152 guide mode. 153

The depth of the dip depends primarily on the length of the 154 metallized section L. The best resolution is achieved with the 155 deepest resonant dip, but if its depth exceeds the dynamic range 156 of the spectrum analyzer employed, the shape of the dip can 157 be distorted by noise. With this in mind we choose the length 158 of the sensing section, in all cases, so that the attenuation at 159 resonance is \sim 80 dB, which corresponds roughly to the dynamic 160 range of a modern optical spectrum analyzer (such as Yokogawa 161 AQ6370D).

To compare metrological performance of different refractometric configuration we thus use the so-called Figure-of-Merit 164 (FOM) parameter defined as the ratio of spectral sensitivity to 165 the logarithmic half-width of the resonant dip. Refractometric 166 resolution is inversely proportional to FOM [6] so the best 167



Fig. 2. Spectral dependencies of the effective refractive index (a) and losses (b) of the hybrid modes of the metallized section, as well as the transmission spectrum of the refractometer (c) at th_m = 60 nm, n_{ext} = 1.4, L = 500 μ m. The insets show MMLS profiles at resonance ($\lambda = 0.703 \ \mu$ m, insets 1, 2) and off resonance ($\lambda = 0.64 \ \mu$ m, insets 3, 4).

SPR-refractometer with the minimum resolution is the one withthe largest FOM value.

Another parameter of an SPR-refractometer, which is im-170 portant for bio- and chemosensing applications, is the penetra-171 tion depth (d_{SP}) of the surface plasmon mode into the ambient 172 medium conventionally defined at the 1/e level of the SPM in-173 tensity profile. That is because the thickness of the sensing layer 174 of ligand molecules (d_{lig}) can be much smaller than d_{sp} . In this 175 case an SPR-refractometer is more appropriately characterized 176 by the so-called local sensitivity: $S_{loc} \propto S_{RI} \frac{d_{lig}}{d_{SP}}$, which takes 177 proper account of the sensitivity of SPM's propagation constant 178 to refractive index variations in a thin layer near the metal film 179 [6]. It then follows that refractometric resolution with respect 180 181 to local RI variations should be proportional to the "local resolution coefficient" (LRC) defined as the ratio of d_{SP} to FOM, 182 which we shall use to compare different SPR-refractometers in 183 terms of local resolution - the smallest LRC value corresponds 184 to the best configuration. 185



III. RESULTS

187 A. SPR-Refractometer Without a Buffer Layer

In practical terms it is advantageous to build an SPR-188 refractometer with the most common and readily available op-189 tical materials, so let us choose SiO₂ ($n_s \sim 1.45$ [20]) as a 190 substrate material and PMMA ($n_w \sim 1.49$ [22]) as a waveguid-191 ing layer material. Numerical calculations then show that for 192 the waveguiding layer thickness th_w = 1.5 μm and ambient re-193 fractive index $n_{ext} = 1.4$ the dispersion curves of the separately 194 considered waveguide and bulk surface plasmon modes inter-195 sect in the near infrared spectral range (Fig. 2a, dotted lines). 196 By the separately considered BSPM we mean the mode of the 197 metal film localized at metal | ambient medium interface, with 198 199 the metal film being bounded on one side by the semi-infinite



Fig. 3. Effective index and loss spectra of hybrid MMLS, transmission spectra of the refractometer, and electric field amplitude distribution in the metallized section at the resonant wavelength at $n_{ext} = 1.4$, $L = 500 \,\mu\text{m}$ and $th_m = 45 \,\text{nm}$ (a), (b), (c), (d), 68 nm (e), (f), (g), (h), 69 nm (i), (j), (k), (l), 74 nm (m), (n), (o), (p).

ambient medium and, on the other side, by semi-infinite di- 200 electric with refractive index n_w . By the separately considered 201 waveguide mode (WM) we mean the single fundamental mode 202 of the waveguiding layer bounded by semi-infinite substrate and semi-infinite ambient medium. 204

According to the coupled mode theory, near the wavelength 205 of intersection of WM and BSPM dispersion curves pronounced 206 losses can occur in Section 2 as a result of transfer of guided 207 light energy to surface plasmons, provided that the WM-BSPM coupling coefficient is sufficiently large. This is indeed the 209 case for the metal film thickness $th_m = 60 \text{ nm}$, which is con-210 firmed by the results of calculation of the effective index spectra 211 (Fig. 2a, solid lines), loss spectra (Fig. 2b) and profiles (insets 1-212 4) of the hybrid modes of multilayer structure (MMLS) forming 213 Section 2. It is evident from insets 1 and 2 that at the resonant 214 wavelength MMLS, with their profiles made up of the elements 215 of both BSPM and WM, are indeed a result of the hybridization 216 of the latter modes. Since both MMLS have similar profiles at 217 this wavelength and, therefore, similar overlap integrals with the 218 waveguide mode of Section 1, they are excited at the beginning 219 of Section 2 with about the same amplitudes. Their losses are 220 equally high ($\sim 1700 \text{ dB/cm}$) and result in the attenuation of 221 guided light power by \sim 80 dB for the length of the metallized 222 section L = 0.5 mm. Off the resonant wavelength, as seen from 223 Fig. 2b and insets 3-4, both profiles and losses of MMLS are 224 quite different. The low loss mode is closer in its profile to the 225 waveguide mode of Section 1 and is, therefore, excited much 226 more efficiently. As a result, there is no significant attenuation 227 of light in Section 2 at this wavelength. It is in this way that a 228 pronounced dip is formed in the transmission spectrum of the 229 refractometer (Fig. 2c). 230

Numerical calculations show that, depending on the thickness 231 of the metal film, the formation of the resonant dip can occur 232 in two distinct scenarios. If the film thickness is 68 nm or less 233 there is an anticrossing in the effective index spectra of hybrid 234 MMLS, and a crossing in their loss spectra. This is illustrated by 235 Fig. 2a, b ($th_m = 60 \text{ nm}$) and Fig. 3a, b, e, f ($th_m = 45; 68 \text{ nm}$). 236 At film thicknesses of 69 nm or more, on the contrary, the MMLS 237 spectra intersect, while their loss spectra do not (Fig. 3i, j, m, n 238 $(th_m = 69, 74 \text{ nm})).$ 239

These scenarios can be associated with two different coupling 240 regimes between the separately considered WM and BSPM. 241 The first scenario can be regarded as strong coupling whereby a 242 243 periodic power exchange takes place at the resonant wavelength between the coupled modes (see also [23] for discussion and 244 [24] for experimental observation of this). This is illustrated by 245 the distribution of the electric field amplitude in Section 2 at a 246 film thickness of 45 nm (Fig. 3d). From the point of view of 247 the entire multilayer structure forming Section 2, this exchange 248 249 corresponds to interference beats of hybrid MMLS with a period of $\lambda/\Delta n$, where Δn is the difference in their effective indexes at 250 the resonant wavelength. Note that this period increases with 251 increasing film thickness and, for example, at $th_m = 68 \text{ nm}$, 252 it becomes larger than the characteristic attenuation length of 253 guided light in Section 2. In this case, the exchange of power 254 between WM and BSPM proceeds too slowly to be seen against 255 the background of the overall attenuation of light in Section 2 256 (Fig. 3h, $th_m = 68 \text{ nm}$). 257

The second hybridization scenario can be associated with a 258 weak-coupling regime in which such a periodic power exchange 259 260 between the waveguide and surface plasmon modes at the resonant wavelength does not occur (see [24] for experimental ob-261 servation of this regime). In terms of MMLS, this corresponds to 262 a situation where interference beats between them are not pos-263 264 sible due to their propagation constants being equal at $\lambda = \lambda_{SPR}$ (Fig. 3i, m). 265

We must emphasize that the terms "strong" and "weak" coupling are understood here differently than in the context of coupling between lossless modes, and both apply to the resonant wavelength where the real parts of the propagation constants of the coupled modes are exactly equal.

It follows from the coupled mode theory [21] that the coupling 271 regime between WM and BSPM is determined by whether or 272 not the coupling coefficient D is larger than the difference of 273 their effective indexes. At the resonant wavelength the latter 274 reduces, due to WM being lossless, to the imaginary part of 275 the BSPM effective index n''_{SP} . If $D > n''_{SP}$, the dependences 276 of the coupled modes amplitudes on the coordinate along the 277 278 fiber can be shown to be quasiperiodic, which corresponds to the strong-coupling regime, and for $D < n''_{SP}$ they acquire a 279 quasi-exponential character corresponding to the weak coupling 280 regime. 281

The coupling coefficient is defined primarily by the thick-282 ness of the metal film: for larger th_m the profiles of WM and 283 BSPM overlap less effectively which leads to lower D value and, 284 therefore, weaker coupling. If the coupling becomes too weak 285 (D << $n^{\prime\prime}{}_{SP}),$ say at $th_m=74\,nm,$ the transfer of guided light 286 energy to surface plasmons becomes inefficient which consid-287 erably reduces the depth of the resonant dip (Fig. 30). In terms 288 289 of MMLS it is explained by the fact that their profiles and losses at the resonant wavelength differ, with lower loss MMLS being 290 291 closer in its profile to the fundamental mode of Section 1. It is, as a result, excited more effectively and to a greater extent 292 affects the overall transmission of the structure, which leads to 293 the observed reduction of the depth of the dip. 294

On the other hand, if the coupling is too strong (D >> n''_{SP}), for example, at th_m = 45 nm, the spectral range around λ_{SPR} where the transfer of energy to surface plasmons is effective



Fig. 4. Calculated transmission spectra of the refractometer for n_{ext} = 1.395–1.41, th_m = 68 nm, L=0.5 mm. Shown in the insets below are the effective index and loss spectra of MMLS of Section 2 at n_{ext} = 1.395; 1.401; 1.406; 1.41.

gets wider, which leads to the broadening of the resonant dip 298 (Fig. 3c). We thus conclude that the sharpest resonant dip is 299 obtained with the critical coupling - just at the border between 300 weak and strong coupling regimes. At $n_{ext} = 1.4$ this is achieved 301 with a film thickness of 68 nm (Fig. 3g). 302

The ambient refractive index, however, does not remain con-303 stant in the course of refractometric measurements. Its varia- 304 tion shifts the resonant wavelength, which, for a fixed value 305 of th_m, is inevitably accompanied by changes in the resonant 306 dip contrast. This is illustrated in Fig. 4 depicting transmission 307 spectra of the refractometer calculated for $th_m = 68 \text{ nm}, n_{ext} =$ 308 1.395-1.41, L = 0.5 mm. As evident from the dispersion curves 309 of hybrid MMLS shown in the insets at the bottom of Fig. 4 the 310 coupling between WM and BSPM gets stronger with increas- 311 ing n_{ext} and λ_{SPR} . This is explained by the fact that, firstly, the 312 profiles of WM and BSPM broaden as the wavelength increases 313 and overlap more effectively thus leading to a larger coupling 314 coefficient. Secondly, n''_{SP} value responsible for the losses of 315 BSPM tend to decrease with increasing wavelength [6], which 316 also makes the coupling stronger. 317

Thus the depth of the resonant dip first gradually growths 318 while shifting from left to right with increasing n_{ext} as the cou- 319 pling gets stronger but is still in the weak coupling regime 320 $(n_{ext} < 1.4)$. The switching to the strong coupling regime oc-321 curs at $n_{ext} \sim 1.4$ after which the coupling continues to grow 322 stronger as seen from the growing difference in the effective 323 indexes of MMLS at the resonant wavelength (marked with 324 arrows in the insets of Fig. 4). At $n_{ext} > 1.4$ one can also ob-325 serve slight quasiperiodic variations in the depth of the resonant 326 dip. They arise from the periodic power exchange between the 327 waveguide and surface plasmon modes resulting into the guided 328 light, depending on the period of the exchange, being predom-329 inantly localized at the end of Section 2 either in the region of 330 the waveguiding layer or near the metal film. This affects the 331 transmission loss between Sections 2 and 3, which varies as the 332



Fig. 5. Effective index spectra for the separately considered waveguide and bulk surface plasmon modes as well as transmission spectra of the refractometer at $th_m = 58 \text{ nm}$, $th_w = 1 \,\mu\text{m}$, L = 0.2 nm, $n_{ext} = 1.34-1.37$ (a), (b) and at $th_m = 75 \text{ nm}$, $th_w = 2.5 \,\mu\text{m}$, L = 1.3 nm, $n_{ext} = 1.433-1.439$ (c), (d). The upper-right inset shows the spectral dependences of losses and depth of penetration of BSPM into the ambient medium.

period of the exchange gets shorter with stronger coupling, thusleading to the observed variations in the depth of the dip.

When the ambient refractive index exceeds \sim 1.406 the resonant dip broadens due to WM-BSPM coupling becoming overly strong and its depth decreases due to lower losses of BSPM at longer wavelengths.

It then seems reasonable to define a range of efficient re-339 fractometric measurements (Δn_{ext}) as the range of n_{ext} values 340 for which the depth of the resonant dip is less than the maxi-341 mum depth by not more than an arbitrary threshold value, say 342 20 dB. For the configuration under study, as seen from Fig. 4, 343 this corresponds roughly to next ranging from 1.395 to 1.41, 344 i.e., $\Delta n_{ext} \cong 0.015$. It also follows from the analysis of the 345 transmission spectra in Fig. 4 that the spectral sensitivity of 346 the refractometer is $S_{RI} \cong 6800 \text{ nm/ RI}$ unit (RIU), logarith-347 mic half-width of the dip in the middle of the measured next 348 range – FWSRM \cong 25 nm. The penetration depth of BSPM into 349 the ambient medium at $\lambda \sim 700$ nm is $d_{sp} \cong 120$ nm (see the 350 inset of Fig. 5), which yields FOM \cong 270 and LRC \cong 0.44. 351

It should be noted that the SPR-refractometer under con-352 sideration can be used for measuring other values of ambient 353 refractive index, both higher and lower than 1.4. For example, 354 at $n_{ext} \sim 1.35$ the phase-matching condition between the wave-355 guide and surface plasmon modes is fulfilled near $\lambda = 550$ nm 356 (Fig. 5a). The optimal film thickness in this case is 58 nm. For 357 the waveguide layer to remain in the single-mode regime its 358 width is reduced to 1 micron. Since the losses of BSPM in this 359 spectral range are several times higher than those at $\lambda \sim 700$ nm 360 (inset of Fig. 5) we also reduce the length of the metallized 361 section to 0.2 mm. 362

In spite of the higher losses of BSPM the width of the resonant dip turns out in this case to be less than in the previous one: FWSRM \cong 16 nm (at n_{ext} \cong 1.35), which can be explained by a much larger angle of intersection of WM and BSPM dispersion curves (Fig. 5a). It is for the same reason that, although physical sensitivity of BSPM's effective index to the ambient RI is larger at shorter wavelengths [6], the overall spectral sensitivity turns out in this case to be about 2.5 times lower 370 than that at $\lambda \sim 700$ nm: S_{RI} $\cong 2600$ nm/RIU due to a drop 371 in the instrumental sensitivity. The rage of measured refractive 372 index is correspondingly larger: $\Delta n_{ext} \cong 0.03$. FOM amounts 373 to ~ 162 which is more than 1.5 times worse than in the previous 374 case. The penetration depth of BSPM into the ambient medium, 375 however, at $\lambda \sim 550$ nm is only ~ 70 nm (inset of Fig. 5), so 376 in terms of the local resolution there is virtually no difference 377 from the previous case: LRC ≈ 0.43 . 378

At a higher value of the ambient refractive index: $n_{ext} \sim 1.435$ 379 the phase-matching condition between the waveguide and sur-380 face plasmon modes is fulfilled at $\lambda \sim 1000$ nm (Fig. 5c). The 381 optimal waveguide width and metal film thickness in this case 382 are 2.5 μ m and 75 nm, respectively. The losses of BSPM in this 383 spectral range are much lower than at $\lambda \sim 700$ nm or $\lambda \sim 550$ nm, 384 so to get a \sim 80 dB resonant dip the length of the metallized sec-385 tion has to be extended to L = 1.3 mm. Secondly, the dispersion 386 curves of WM and BSPM intersect here at a much smaller an-387 gle than in both cases considered above. This leads to a much 388 higher spectral sensitivity due to a larger instrumental contri-389 bution: $S_{RI} \cong 26000 \text{ nm/ RIU}$, narrowing of the measured RI 390 range: $\Delta n_{ext} \cong 0,008$, and broadening of the resonant dip. The 391 latter feature is, however, partially compensated by the lower 392 losses of BSPM in this spectral range resulting in FWSRM \cong 393 44 nm (at $n_{ext} \approx 1.435$). There is thus a significant advantage 394 in terms combination of spectral sensitivity and width of the dip 395 as compared to the previous cases: FOM \cong 590. The local reso-396 lution is, however, virtually unchanged because of much deeper 397 penetration of BSPM into the ambient medium at $\lambda \sim 1000$ nm 398 $(d_{SP} \cong 270 \text{ nm}, \text{ inset of Fig. 5})$: LRC $\cong 0.46$. 399

B. SPR-Refractometer Based on Symmetric (Long-Range)400Surface Plasmon Mode401

Introduction of a buffer layer between the waveguide and 402 metal film with the refractive index close to that of the am-403 bient medium enables one to build an SPR-refractometer both 404 on symmetric (long-range) and antisymmetric (short-range) sur-405 face plasmon modes [6]. SSPM and ASPM differ significantly in 406 their properties both from each other and from the bulk surface 407 plasmon mode considered above. The metrological parameters 408 of corresponding SPR-refractometers can, therefore, be widely 409 different as well. To gain a benefit in metrological performance 410 one must to the fullest possible extent exploit the advantages 411 that a particular plasmon mode has to offer in terms of building 412 an SPR-refractometer. 413

As for the long-range surface plasmon mode its major strength 414 is in its low propagation losses [6], [15]–[17]. This enables one 415 to obtain a reasonably narrow resonant dip even with a very 416 small intersection angle between WM and SSPM dispersion 417 curves, which may yield a very high spectral sensitivity due 418 to a large instrumental contribution. The losses of SSPM tend 419 to decrease for larger wavelength and thinner metal film [6], 420 which makes it reasonable to use a long-wavelength spectral 421 range and a thin metal film. Making the film too thin, how-422 ever, is not practical and can be technologically challenging. 423 At too long a wavelength, on the other hand, the intersection 424 angle can become too small to produce a distinct resonant dip 425



Fig. 6. Dispersion curves of the separately considered waveguide and symmetric surface plasmon modes (a) and transmission spectra of the SSPM-based refractometer (d) for $n_{ext} = 1.3299-1.3302$; effective index and loss spectra of the hybrid MMLS of the metallized section for $n_{ext} = 1.3299$ (b), (e) and 1.33 (c), (f) (L = 60 mm, th_w = 200 nm, th_b = 13.3 μ m, th_m = 20 nm).

in spite of SSPM's low losses. With thus choose as a com-426 promise th_m = 20 nm and $\lambda \sim 1000$ nm. We note also that the 427 effective index of the long-range surface plasmon mode is much 428 lower than those of ASPM and BSPM, so to phase-match it to 429 430 the waveguide mode one has to use materials with low optical density. The specified requirements are fulfilled e.g., with the 431 following waveguiding structure: substrate made of Cytop poly-432 mer ($n_s \sim 1.34$ [25]), waveguiding layer – MgF₂ ($n_w \sim 1.37$ [26], 433 434 $th_w = 200 \text{ nm}$), buffer layer – Cytop, silver film ($th_m = 20 \text{ nm}$).

Fig. 6a shows the dispersion curves of the separately con-435 sidered WM and SSPM calculated for the chosen structure at 436 $n_{ext} = 1.33$. As seen from the figure the phase-matching be-437 tween the two modes can be achieved near $\lambda = 1040$ nm. To 438 ensure the maximum contrast of the resonant dip we also re-439 440 quire the switching from the weak to strong regime of WM-SSPM coupling to occur around this wavelength. Unlike the 441 previously considered configuration, in the SPR-refractometer 442 with a buffer layer it is the thickness of the buffer layer that is 443 primarily responsible for the coupling regime. Calculation show 444 that the optimal value of th_b at which the switching of coupling 445 regimes occurs near $\lambda = 1040$ at $n_{ext} \approx 1.33$ amounts to 13.3 446 microns (Fig. 6b, c, e, f). 447

The transmission spectra of the refractometer calculated 448 for $n_{ext} = 1.3299 - 1.3302$, th_b = 13.3 μ m are shown in Fig. 6d. 449 One can conclude from the figure that spectral sensitiv-450 ity in this case amounts to as high as ~ 120000 nm/RIU, 451 $\Delta n_{ext} \cong 0,0004$, FWSRM $\cong 18$ nm (at $n_{ext} \cong 1.3301$), i.e., 452 FOM \cong 6670, which is more than an order of magnitude 453 higher than that of the SPR-refractometer without a buffer 454 layer. In spite of the penetration depth of SSPM into the 455 ambient medium being much higher than that of BSPM 456 $(d_{SP} \cong 580 \text{ nm at } \lambda \sim 1050 \text{ nm})$ in terms of local resolution 457 the SPR-refractometer based on SSPM has a significant advan-458 tage as well: LRC \cong 0.09 which is ~5 times below that of 459 SPR-refractometer without a buffer layer. We must note, how-460 461 ever, that the advantage in metrological performance arises from the low losses of SSPM (~30 dB/cm at $\lambda \sim 1050$ nm) and it 462 comes, therefore, at a cost of extending the length of the sensing 463 section: an \sim 80dB resonant dip is achieved with the sensing 464 section being as long as 6 cm. 465

If needed the sensing section can be shortened by choosing the parameters of the structure so that the SPR condition is fulfilled at a shorter wavelength where SSPM has higher losses. 468 For example, at $th_w = 400 \text{ nm}$ and $n_{ext} = 1.33$ the waveguide 469 mode is phase-matched to SSPM at around $\lambda = 600$ nm. The 470 optimal thickness of the buffer layer is $th_b = 2.6 \,\mu m$. The 471 losses of SSPM in this spectral range are about an order of 472 magnitude higher than those at $\lambda \sim 1000$ nm: ~ 310 dB/cm 473 enabling 10-fold shortening of the sensing section: L = 6 mm. 474 The spectral sensitivity, however, turns out in this case to be 475 only about a tenth of that at $\lambda \sim 1000$ nm due to a sharp 476 drop in the instrumental contribution: $S_{RI} \cong 16000 \text{ nm/ RIU}, 477$ which is accompanied by broadening of the RI measurement 478 range: $\Delta n_{ext} \cong 0.003$ and some narrowing of the resonant dip: 479 FWSRM \cong 12 nm. Thus, in terms of combination of sensitivity 480 and resonant dip width such a configuration is more than 5 times 481 inferior to the previous one: FOM \cong 1330. The local resolution 482 is, however, not much worse than that in the previous case due 483 to much a lower penetration depth of SSPM at $\lambda \sim 600$ nm 484 than at $\lambda \sim 1000$ nm (d_{sp} $\cong 200$ nm): LRC $\cong 0.15$. 485

C. SPR-Refractometer Based on the Antisymmetric 486 (Short-Range) Surface Plasmon Mode 487

From the analysis of the properties of the antisymmetric sur- 488 face plasmon mode [6] one can conclude that its main advan- 489 tages in terms of building an SPR refractometer are as follows. 490 Firstly, it has a higher degree of field localization near the film 491 which may lead to better sensitivity to local variations of refrac- 492 tive index. Secondly, it has a higher physical sensitivity to the 493 ambient refractive index as compared to SSPM. Thirdly, higher 494 losses of ASPM allow one to obtain a deep resonant dip with a 495 very short sensing section, which aids in miniaturization of the 496 refractometer. All of these features become more pronounced 497 with decreasing wavelength and metal film thickness [6]. An- 498 other circumstance to take into account is that, as calculations 499 show, when the media on two sides of the film differ in refrac- 500 tive indexes the profile of ASPM tends to shift to the optically 501 denser medium, which brings about additional increase in sen- 502 sitivity to the refractive index of that medium. Thus in order to 503 exploit ASPM's advantages to the fullest degree one should use 504 shorter wavelength range, very thin film and make the refractive 505 index of the buffer layer somewhat lower than that of the am- 506 bient medium. Due to the effective index of ASPM being quite 507 high [6], to enable its phase-matching with the waveguide mode 508 one should use for the waveguiding layer a high optical density 509 material. 510

The stated requirements are satisfied e.g., with the following 511 structure: substrate – SiO₂, waveguiding layer – Si₃N₄ ($n_w \sim 2$ 512 [27], th_w = 250 nm), buffer layer – Teflon AF2400 ($n_b \sim 1.28$ 513 [28]), silver film (th_m = 20 nm), ambient medium ($n_{ext} > n_b$). 514

Fig. 7a shows the dispersion curves of the separately 515 considered waveguide and antisymmetric plasmon modes 516 calculated for the chosen structure at different n_{ext} values in 517 the range 1.34–1.37. As one can see, the SPR condition is 518 fulfilled at $\lambda \sim 640$ nm where ASPM losses are found to be 519 as high as ~42000 dB/cm. The optimal thickness of the buffer 520 layer at which the switching of WM-ASPM coupling regimes 521 occurs near this wavelength is th_b = 180 nm (Fig. 7b, c, e, f). 522 The losses of hybrid MMLS at the resonant wavelength reach 523

	SPR-refractometer without a buffer layer			SPR-refractometer based on long- range surface plasmon mode		SPR-refractometer based on short- range surface plasmon mode	
Measured RI, $\overline{n_{ext}} \pm \frac{\Delta n_{ext}}{2}$	1.355±0.015	1.404±0.0075	1.437±0.004	1.33±0.0015	1.3301±0.0002	1.355±0.015	1.33±0.01
Resonant wavelength range, nm	530-610	680-780	920-1120	600-650	1030-1080	625-655	900-980
Instrumental sensitivity, S1	2 000	6 000	24 000	34 000	316 000	825	4 350
Physical sensitivity, S ₂	1.26	1.14	1.08	0.47	0.38	1.09	0.85
Spectral sensitivity S _{RI} , nm/RIU	2 600	6 800	26 000	16 000	120 000	900	3 700
FWSRM, nm	16	25	44	12	18	35	65
FOM	162	270	590	1 330	6 670	25,7	57
SPM losses near λ_{SPR} , dB/cm	11 620	3 650	970	310	30	42 000	11 000
Length of the sensing section, mm	0.2	0.5	1.3	6	60	0.04	0.18
SPM penetration, d _{SP,} nm	70	120	270	200	580	44	117
Local resolution coefficient, LRC	0.43	0.44	0.46	0.15	0.09	1.7	2.05

 TABLE I

 Specifications of the SPR-Refractometers Under Study



Fig. 7. Dispersion curves of the separately considered waveguide and antisymmetric surface plasmon modes (a), as well as transmission spectra of the ASPM-based refractometer (d) calculated for $n_{ext} = 1.34-1.37$; effective index and loss spectra of hybrid MMLS of the metallized section calculated for $n_{ext} = 1.37$ (b), (e) and 1.35 (c), (f) (L = 0.04 mm, th_w = 250 nm, th_b = 180 nm, th_m = 20 nm).

524 ~22 000 dB/cm which makes it possible to reduce the length 525 of the sensing section to just $L = 40 \ \mu m$.

The transmission spectra of the refractometer are shown 526 in Fig. 7d. It can be concluded from the figure that the 527 spectral sensitivity is in this case \sim 900 nm/RIU, $\Delta n_{ext} \cong$ 528 0.03, FWSRM \cong 35 nm (at n_{ext} \cong 1.36), and FOM \cong 25.7, 529 which is about an order of magnitude lower than the FOM of the 530 refractometer without a buffer layer and 260 times lower than 531 the FOM of the refractometer on SSPM. The penetration depth 532 of ASPM into the ambient medium, however, at $\lambda \sim 640$ nm is 533 just \sim 44 nm and LRC amounts, therefore, to \sim 1.7. 534

We note that such a low sensitivity results from an extraordi-535 narily low instrumental contribution due to a very large intersec-536 tion angle of WM and ASPM dispersion curves. The parameters 537 of the waveguiding structure can be adjusted to shift the reso-538 nance to a longer wavelength thus decreasing the intersection an-539 gle and enhancing the sensitivity. This will also broaden the res-540 onant dip but due to ASPM losses falling with wavelength some 541 benefit should be expected in terms of FOM parameter (at the ex-542 pense of a longer sensing section). For example, at $th_b = 150 \text{ nm}$ 543 and $n_{ext} \sim 1.33$ the SPR condition is fulfilled at $\lambda \sim 900$ nm 544 where the losses of ASPM amount to ~ 11000 dB/cm. At 545 546 the optimal film thickness ($th_b = 568 \text{ nm}$) an 80-dB resonant dip can be obtained with a sensing section of 180 μ m. 547 The spectral sensitivity is then found to be ~3700 nm/RIU, 548 $\Delta n_{ext} \cong 0.02$, FWSRM $\cong 65$ nm, $d_{SP} \cong 117$ nm, which results in FOM $\cong 57$ and LRC $\cong 2.05$. 550

IV. DISCUSSION 551

The specifications of the studied BSPM, SSPM- and ASPMbased refractometers are summarized in Table I. As seen from the table the difference in metrological performance of different configurations results mainly from their spectral sensitivity. The physical sensitivity, however, does not change much and the observed variations are primarily due to the greatly varying instrumental contribution.

The best specifications are achieved with the SPR-559 refractometer based on symmetric or long-range surface plas-560 mon mode: due to its low losses a sharp resonant dip can be 561 obtained even with a very small intersection angle of WM and 562 SSPM dispersion curves yielding an extremely high instrumen-563 tal and hence overall spectral sensitivity. The advantage in terms 564 of FOM parameter reaches about two orders of magnitude as 565 compared to the ASPM-based SPR-refractometer and one order 566 of magnitude as compared to the SPR-refractometer without a 567 buffer layer. 568

Apart from its low losses the symmetric surface plasmon 569 mode has a larger penetration depth into the ambient medium. 570 In terms of local resolution, therefore, the advantage of using 571 SSPM instead of ASPM or BSPM is less pronounced: LRC is 572 about 20 times lower than that for ASPM and ~6 times lower 573 than that for BSPM. 574

We should also emphasize that the advantage in metrological 575 performance of the SPR-refractometer based on symmetric surface plasmon mode comes at a cost of extending the length of the 577 metallized section: to obtain a resonant dip of the same depth as 578 in ASPM- and BSPM-based refractometers a much longer (up 579 to three orders of magnitude) sensing section is required. 580

The most compact sensing element with the minimum length 581 of the sensing section is characteristic of the SPR-refractometer 582 based on the antisymmetric surface plasmon mode. It has, 583 584 however, the worst metrological performance among all the 585 studied configurations due to the enormous losses of ASPM.

The SPR-refractometer without a buffer layer occupies an intermediate position between those based on SSPM and ASPM, both in terms of metrological performance and sensing section length. It has, however, an important practical advantage of having the simplest structure, which facilitates the fabrication process.

One can also conclude from the table that the values of 592 593 measured refractive index depend both on the parameters of the metallized section and on the working spectral range. By 594 choosing a longer wavelength range where a surface plasmon 595 mode has lower losses (and using a longer sensing section) one 596 can obtain higher metrological performance in terms of FOM 597 parameter. The local resolution coefficient, however, does not 598 change much since the increase in FOM is offset by a higher 599 penetration depth of SPM into the ambient medium. We also 600 note that if the resonant wavelength is shifted too far into the 601 infrared ($\lambda_{\text{SPR}} \gtrsim 1200 \text{ nm}$) the intersection angle between WM 602 and SPM dispersion curves may get so small that refractometric 603 measurements, in spite of a very high sensitivity, become no 604 605 longer possible due to smearing out of the resonant dip.

In closing, we emphasize that metrological parameters sum-606 marized in Table I have been obtained in the 2D-geometry 607 608 approximation and depend on the specific choices of materials and geometric parameters of the refractometers. Their pri-609 mary purpose is, therefore, not to characterize performance of 610 practical SPR-sensors but to illustrate in a quantitative manner 611 the relative merits of refractometers based on bulk, symmet-612 ric and antisymmetric surface plasmon modes. The revealed 613 614 patterns and relationships, we believe, are also valid in 3D geometry and do not depend on the specific details of the 615 refractometers. 616

V. Co

V. CONCLUSIONS

We have thus studied three SPR-refractometer configurations: 618 without a buffer layer based on the excitation of the bulk sur-619 face plasmon mode, and with a buffer layer using symmetric 620 (long-range) and antisymmetric (short-range) surface plasmon 621 622 modes. It is shown the highest metrological performance is achieved with the symmetric SPM, which, however, requires a 623 much longer sensing section. If miniaturization of the sensor is 624 of utmost importance the preferred type of plasmon mode to 625 use is the antisymmetric one, which enables minimization of 626 the sensing section length at a cost of impaired metrological 627 specifications. Finally, in terms of ease of fabrication the most 628 attractive configuration is that without a buffer layer, which is 629 630 intermediate between SSPM- and ASPM-based refractometers both in terms of metrological performance and sensing section 631 632 length.

633

617

References

- [1] A. Rasooly and K. E. Herold, *Biosensors and Biodetection*. New York,
 NY, USA: Humana, 2009.
- [2] Ligler F. S. and C. R. Taitt, *Optical Biosensors: Today and Tomorrow.* Amsterdam, The Netherlands: Elsevier, 2011.

- Science & Business Media, 2006, vol. 224.
 639

 [4] X. Guo and J. Biophoton, "Surface plasmon resonance based biosensor technique: A review," J. Biophoton., vol. 5, pp. 483–501, 2012.
 641
- [5] J. Homola, "Surface plasmon resonance sensors for detection of chemical and biological species," *Chem. Rev.*, vol. 108, no. 2, pp. 462–493, 2008. 643
- [6] J. Homola, Surface Plasmon Resonance Based Sensors. Berlin, Germany: 644 Springer-Verlag, 2006. 645
- [7] B. D. Gupta and R. K. Verma "Surface plasmon resonance-based fiber 646 optic sensors: Principle, probe designs, and some applications," *J. Sensors*, vol. 2009, 2009, Art. no. 979761.
- [8] R. Kashyap and G. Nemova, "Surface plasmon resonance-based fiber and 649 planar waveguide sensors," J. Sensors, vol. 2009, 2009, Art. no. 645162. 650
- [9] C. Caucheteur, T. Guo, and J. Albert "Review of plasmonic fiber optic biochemical sensors: Improving the limit of detection," *Analytical Bioanalytical Chem.*, vol. 407, no. 14, pp. 3883–3897, 2015.
- [10] E. Klantsataya *et al.*, "Plasmonic fiber optic refractometric sensors: From 654 conventional architectures to recent design trends," *Sensors*, vol. 17, no. 1, 655 2016, Art. no. 12.
- S. K. Srivastava and B. D. Gupta, "Fiber optic plasmonic sensors: Past, present and future," *Open Optics J.*, vol. 7, no. 1, pp. 58–83, 2013.
- M. E. Bosch *et al.*, "Recent development in optical fiber biosensors," 659 Sensors, vol. 7, no. 6, pp. 797–859, 2007.
- [13] A. V. Dyshlyuk *et al.*, "Numerical and experimental investigation of 661 surface plasmon resonance excitation using whispering gallery modes in 662 bent metal-clad single-mode optical fiber," *J. Lightw. Technol.*, vol. 35, 663 no. 24, pp. 5425–5431, Dec. 2017.
- [14] Y.-S. Chu *et al.*, "Surface plasmon resonance sensors using silica-onsilicon optical waveguides," *Microw. Opt. Technol. Lett.*, vol. 48, no. 5, pp. 955–957, 2006.
- [15] G. G. Nenninger *et al.*, "Long-range surface plasmons for high-resolution surface plasmon resonance sensors," *Sensors Actuators B: Chem.*, vol. 74, no. 1–3, pp. 145–151, 2001.
- [16] R. Slavík and J. Homola, "Ultrahigh resolution long range surface 671 plasmon-based sensor," *Sensors Actuators B: Chem.*, vol. 123, no. 1, 672 pp. 10–12, 2007.
- [17] J. Dostálek, A. Kasry, and W. Knoll, "Long range surface plasmons for observation of biomolecular binding events at metallic surfaces," *Plasmonics*, vol. 2, no. 3, pp. 97–106, 2007.
- [18] B. Fan, F. Liu, Y. Li, Y. Huang, Y. Miura, and D. Ohnishi, "Refractive 677 index sensor based on hybrid coupler with short-range surface plasmon 678 polariton and dielectric waveguide," *Appl. Phys. Lett.*, vol. 100, no. 11, 679 2012, Art. no. 111108.
- B. Fan *et al.*, "Integrated refractive index sensor based on hybrid coupler 681 with short range surface plasmon polariton and dielectric waveguide," 682 *Sensors Actuators B: Chem.*, vol. 186, pp. 495–505, 2013.
- [20] E. D. Palik Handbook of Optical Constants of Solids. New York, NY, 684 USA: Academic, 1998.
 685
- [21] A. W. Snyder and J. Love *Optical Waveguide Theory*. Berlin, Germany: 686 Springer Science & Business Media, 2012. 687
- [22] N. Sultanova, S. Kasarova, and I. Nikolov, "Dispersion properties of optical polymers," *Acta Physica Polonica-Series A Gen. Phys.*, vol. 116, no. 4, pp. 585–587, 2009.
- M. L. Nesterov, A. V. Kats, and S. K. Turitsyn, "Extremely short-length 691 surface plasmon resonance devices," *Optics Express* vol. 16, no. 25, 692 pp. 20227–20240, 2008.
- [24] H. Ditlbacher *et al.*, "Coupling dielectric waveguide modes to surface 694 plasmon polaritons," *Opt. Express*, vol. 16, no. 14, pp. 10455–10464, 695 2008.
- [25] 2018. [Online]. Available: http://www.bellexinternational.com/products/ 697
 cytop/pdf/cytop-catalog.pdf
 698
- [26] H. H. Li, "Refractive index of alkaline earth halides and its wavelength 699 and temperature derivatives," J. Phys. Chem. Ref. Data, vol. 9, no. 1, 700 pp. 161–290, 1980.
- [27] H. R. Philipp, "Optical properties of silicon nitride," J. Electrochemical 702 Soc., vol. 120, no. 2, pp. 295–300, 1973.
 703
- [28] M. K. Yang, R. H. French, and E. W. Tokarsky, "Optical properties 704 of Teflon AF amorphous fluoropolymers," *J. Micro/Nanolithography*, 705 *MEMS*, *MOEMS*, vol. 7, no. 3, 2008, Art. no. 033010. 706

638