

RCWA/aRCWA – An Efficient and Diligent Workhorse for Nanophotonic/Nanoplasmonic Simulations – Can it Work Even Better?

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ABSTRACT

In this contribution, fundamentals of both periodic rigorous coupled wave analysis (RCWA) technique as well as aperiodic (aRCWA) techniques will be reviewed, starting with standard algorithms and following with their important as well as alternative extensions and ingredients. Although today, these methods are also often called Fourier modal methods (FMM), we would prefer here their original name stemming from the diffraction grating analysis. The importance of these frequency-domain rigorous techniques has been even increased, as a plethora of novel designs of nanophotonic and nanoplasmonic structures is increasingly growing, not only bringing new physics into life, but also attracting photonics devices applications. As had been demonstrated, the original periodic RCWA method has become applicable also to modeling isolated structures, as photonic waveguides and cavities; these isolated objects being considered as a single period of “supergrating”, with a proper separation of neighboring “superperiods” in contrast to coupling in standard periodic structures. The extensions and ingredients primarily include, mostly, e.g. various correct (or fast) Fourier factorization schemes, adaptive spatial resolution techniques, symmetry considerations, incorporation of general fully anisotropic materials, as well as various variants of boundary conditions and correct field calculation procedures. Finally, several alternative approaches / modifications to several critical parts within the algorithm, which can improve the algorithm performance, in terms of time efficiency and / or computational requirements, will be presented. In previous couple of years, we have developed in-house 2D and 3D numerical tools based on RCWA / aRCWA methods for the analysis of nanophotonic and nanoplasmonic structures and systems. Also, such technical issues as computational capabilities, algorithm speed, memory and time requirements, and possibilities for their optimization in terms of partial or even more pronounced improvements will be mentioned, too. These modeling techniques have significantly helped to the analysis of various subwavelength structures we have performed recently. Here, only two selected simulation problems will be discussed: (1) Bragg structures based on SWG structured waveguides, and (2) plasmonic arrayed structures with lattice resonances.

Keywords: numerical modeling, Fourier modal method, rigorous coupled wave analysis, subwavelength photonic structure, plasmonic structure, Fourier factorization, adaptive spatial resolution, scattering matrix.

1. INTRODUCTION

This paper is intended to report on our numerical simulation techniques we had developed within the last years, based on RCWA/aRCWA frequency-domain Fourier modal techniques, applicable to simulations of general 3D nanophotonic and nanoplasmonic structures of interest. Today, numerical modeling clearly represents an inseparable and perhaps most important part of the analysis and design process of novel photonic structures and devices. Despite the tremendous progress in computational power and memory of modern computers, realistic 3D modeling still remains rather challenging. Apart from direct numerical methods (relying on a direct discretization in the form of differences or elements), modal methods, representing the fields in various modal bases, have their advantages. These Fourier expansion methods model optical field distribution in structures as a specific scattering problem, with a given wave impinging on a structure, calculating the resulting total field distribution. For 3D structures, a fundamental modeling task relies on the way how a sufficiently large number of rigorously calculated 2D eigenmodes are calculated in each uniform section.

The structure of this paper is as follows, Section 2 contains brief overview of our advanced in-house numerical modal techniques based on the RCWA/aRCWA techniques. Here, first, the fundamentals and essentials of the algorithm are first shown. Then, the attention is also given to the issue of applicable boundary conditions, some special techniques improving the algorithm performance, and a critical consideration of recent developments and future prospects. The paper is summarized with the conclusion in Section 4.

2. RCWA/aRCWA ALGORITHMS

2.1 Fundamentals of RCWA/aRCWA Techniques

Methods utilizing Fourier expansion of optical fields were – quite naturally – initially developed for modeling light diffraction by gratings. To stress the difference from the classical coupled wave theory, the term “rigorous coupled wave analysis” (RCWA) was introduced by Moharam and Gaylord in early eighties [1]. In RCWA the eigenmodes are obtained more easily than in the coupled wave techniques, with the help of Fourier expansion into spatial harmonics as a matrix eigenvalue problem. However, it took more than a decade until a bad convergence of TM-polarized fields for metallic gratings initiated, first based on intuitive arguments, a modification of the formalism known lately as “proper Fourier factorization” [2], and further extended to more complicated geometries, anisotropic materials, and crossed (2D) gratings. About a 15 years ago, this approach started to be applied also to modeling photonic waveguides [3]. In this approach (referred as aperiodic RCWA, aRCWA), the waveguide is considered as a single “superperiod” of the grating, and neighboring waveguides – grooves – are mutually isolated by artificially introduced boundary conditions, see section 2.2. Examples for 2D and 3D structures are shown in Figures 1a and 1b, respectively.

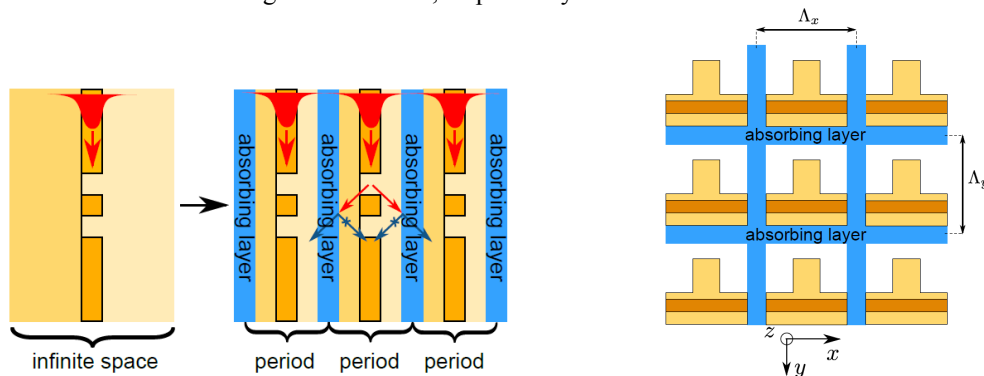


Figure 1. Schematic picture of aRCWA principles: (a) simulation of 2D structures with 1D artificial periodization, (b) simulation of 3D structures with 2D artificial periodization.

When simulating structures with nonrectangular features, further extensions of Li’s correct Fourier factorization schemes, were extended to such cases, including normal vector method (NVM) [4] and its modifications based on complex polarization bases.

In this way, in our laboratory, RCWA/aRCWA codes were developed, including all efficient up-to-date techniques. The solver was further supplemented with the effective propagation algorithms, based on advanced schemes of numerically-stable matrices. Clearly, for analyzing the whole structures, matching the boundary conditions at the interfaces between individual sublayers of the structure must be completed. Within modal methods in general, matrix algorithms are typically used to obtain the solution, with several concepts introduced: (enhanced) transfer matrix (T-matrix) algorithm [5], scattering matrix (S-matrix) algorithm [6], and others (R-matrix and other modifications). While the numerically unstable standard transfer matrix algorithm relates known forward and backward propagating fields at the input to unknown forward and backward propagating fields at the output, the numerical stable scattering matrix represents essentially a 4 port system separating the information on one-side (known system inputs) from the opposite side (unknown system outputs). However, the numerical instability of the T-matrix can be overcome with its enhanced version [5]. We have successfully implemented and compared both enhanced T-matrix and S-matrix algorithms, with practically equivalent performance.

Moreover, we have also developed a specific extension of the aRCWA tool, a fully anisotropic code (including general form of anisotropy of both permittivity and permeability) in 2D, called magnetooptic RCWA/aRCWA (MORCWA/MOaRCWA), since it has found its main application in the analysis of advanced MO structures with non-reciprocal properties.

2.2 Boundary Conditions

As was noted, to simulate a single photonic structure using the RCWA method, it is necessary to insert the artificial absorbing layers between adjacent periods, in order to separate the periods. Such absorbing layers should minimize backward parasitic reflections into the investigated structure, for any wavelength, angle, or polarization. For the aRCWA, perfectly matched layers (PML) [7], as an artificial “absorbing” layer used to truncate computational regions, appears as an appropriate choice. In fact, the concept of PMLs in aRCWA can be introduced in a variety of ways, using a complex coordinate stretching [8], or a anisotropic uniaxial medium [9], or a nonlinear complex coordinate transformation [10]. Concerning the nonlinear complex coordinate transformation approach, here, the computational space is divided into three subintervals; the absorption of the outgoing waves occurs in the first and the third interval (outer layers) due to the nonlinear and complex space,

while the space in the second interval is linear non-complex (non-absorbing). Then, the eigenvalue problem is reformulated in terms of new coordinates. For the case of a uniaxial perfectly matched layer implementation, the material is assumed to be diagonally anisotropic. In this case, the PML layer is characterized by one complex number. Indeed, we confirmed with successful implementation and application that both these transformations ensure the effective isolation of neighboring periods, by both these types of boundary condition.

2.3 Improvements and Specialties

To further enhance the algorithm performance, several specialized add-on techniques, either improving the feasibility of calculations, or enabling the computation under specific conditions, are suitable to implement. According to our experience, one of the most important improvement techniques appears the adaptive spatial resolution (ASR) technique (see, e.g. [11,12]). It is aimed at reducing the Gibbs phenomenon around the permittivity discontinuities, improving the convergence of the Fourier series within the algorithm. Actually, several conceptually different approaches have emerged. The simplest one tries to find suitable analytical coordinate transformations which would reduce the Gibbs overshooting effect. The transformation exchanges the original coordinate to a new smooth one, with typically one control parameter (stretching coefficient), for tuning and optimizing the ASR performance (typically, a step-index permittivity profile is converted into a harmonic-type profile). In fact, we have also contributed to this issue, proposing another ASR transformation function [13]. This transformation leaves the former PML transformation intact, our ASR function is chosen to be linear with the unity slope and smooth at both PML boundaries. Clearly, depending on the algorithm dimensionality, one or two coordinate transformations in orthogonal directions are applied.

Next, in combination with the ASR, structural symmetries for fully 3D problems are also applied. In this case, there is a limitation on the number of orders that can be retained in any given computation, given with both physical restraints (amount of computer memory) and computational time. As it turns out, however, when a structure to be modeled possesses proper symmetries (structural symmetry as well as input wave symmetry – i.e. a mirror symmetry along the x-axis, y-axis, or combined - (x + y)-axis symmetry, also called C_{2v} symmetry), both these issues can be reduced by taking advantage of these symmetries. Our interest has been directed to these symmetries, although other types of symmetries (e.g. C₄, C_{4v} symmetries) can be introduced into the RCWA method, too. For our case, utilizing the symmetry conditions for the wave amplitudes, the relevant matrices for the eigenvalue problem can be dramatically reduced (from $2(2N+1)^2$ to $(2N+1)^2$ only, in one direction), further reducing both memory requirements as well as calculation times (by a factor of 64 for both orthogonal symmetries).

Calculation of Bloch modes. In case of repeated equivalent regions within the analyzed structures of interest, one can first simply use the fact that any interconnection of two S-matrices is again a S-matrix (Redheffer's star product). However, for periodic structures, Bloch mode concept, based on the Bloch's theorem, is more appropriate and efficient (note that Bloch modes represent solutions of the Maxwell's equations in periodic media). This concept has been added to our algorithm to enable stable calculations and handling of Bloch waves, inherent to a proper physical description. Actually, the S-matrix method, mentioned above, may also be used for a proper calculation of fundamental Bloch modes (or, more precisely, their effective indices), leading to a generalized eigenproblem equation.

2.4 Recent Progress of RCWA/aRCWA Algorithms

As presented above, although it might have seemed that the research on RCWA/aRCWA is finished, the opposite is true. Even though the major issues, especially in connection to convergence, time and hardware efficiency, have been settled, recently, a number of specific algorithms improvements and enhancement have appeared. These are taking up on importance since many novel designs of complex photonic and/or plasmonic nanostructures are constantly emerging, in close connection to photonics devices applications. Thus, within the FMM community, various alternative approaches / modifications to several critical parts within the algorithm have appeared, potentially showing either partial or even strong improvement in terms of performance / time efficiency and capabilities. We have also partially contributed to these issues. In this manner, substitutions (non-Fourier) to standard Fourier expansions have been questioned, starting with the Legendre [14] or Gegenbauer polynomials [15], or B-spline functions [16]. Increased needs for efficient treatment of various structures with dramatically different material / geometrical components has led to, e.g. the applications of non-cartesian coordinates [17,18], special boundary conditions enabling to simulate zero dimensional structural parts (such as graphene ribbons) [19]. Also, with increasing interest in nonlinear optical effects, some have been implemented within the RCWA algorithm [20,21], although it is known that the implementation is in principle quite inefficient. Finally, recent attention has been devoted to issues connected with general convergence issues, or, the treatment of nonconvergence with the RCWA algorithm [22,23]. Although these studies showed that, under some rather specific conditions, the algorithm fails to converge, fortunately, these specific conditions are almost not met in practice. To conclude, as was demonstrated, there is still a plenty of room left to make the algorithms work even better and more efficiently, answering the question from the title positively.

3. TWO SELECTED ADVANCED SIMULATION EXAMPLES

In this part, we present a short twofold selection of our new results obtained in two selective categories only while, during last years, we have been active in a much broader simulation activities, applying our RCWA/aRCWA techniques. Thus, the structures of our interest in the theoretical analysis and numerical modeling have ranged from advanced plasmonic guiding structures (such as novel hybrid dielectric plasmonic slot waveguides), surface plasmon resonance structures, nonlinear plasmonic couplers, 3D resonant nanostructures, plasmon-based structures with extraordinary optical transmission effects, negative-index metamaterials, and 3D synthetic opal photonic crystals. These, together with the two study problems, discussed below, namely: (1) Bragg structures based on SWG structured waveguides, and (2) plasmonic arrayed structures with lattice resonances.

3.1 SWG Bragg Waveguide Structures

Recently, it has begun clear that subwavelength grating (SWG) waveguides represent a flexible and perspective alternative to standard silicon-on-insulator nanophotonic waveguides [33-38]. In contrast to standard nanowire waveguides with longitudinal uniformity, prone to rather high scattering losses due to surface roughness, in SWG structures, the field can propagate in the form of Bloch modes. One of the main advantages of such structures is a relatively simple tunability of design parameters enabling a broad variability of the (effective) refractive index and its dispersion, with simultaneous preservation of technological and fabrication demands. In this way, SWG waveguides can indeed provide a promising alternative to standard nanophotonic platform, due to a variety of signal processing functions provided with tunability of SWG waveguide structure parameters. To enable functionality, a SWG waveguide has to be designed with a period (much) smaller than the operational wavelength of light, each period composed of a rectangular silicon nanoblock, embedded into a lower-index superstrate. Clearly, one of the main tuning parameters is the filling factor, i.e., the duty-cycle of the SWG structure.

Although several classes of such structures (straight guides, tapers, crosses, mode transformers and converters, ring resonators, MMI couplers, or even Bragg gratings) have been described and fabricated, we have shown, using our rigorous 3D modeling tools, that an effective 2D approach, often applied in such situations, is totally inadequate [29]. Then, we have investigated several integrated-optic components based on spatially segmented SWG waveguides, with our numerical techniques, extended towards the Bloch mode calculations. These activities have been performed in cooperation with P. Cheben (National Research Council, Ottawa, Canada) where these structures are being intensively researched, especially experimentally. Additionally, we have succeeded in determining the operating spectral regions and the dispersion properties (phase and group indices), confirming the flexibility of SWG structures with respect to design parameters [30]. Moreover, we accomplished a study analysis of the properties of SWG mode converters (tapers) designed for efficient excitation of a SWG waveguide from / to a standard silicon nanowire [31].

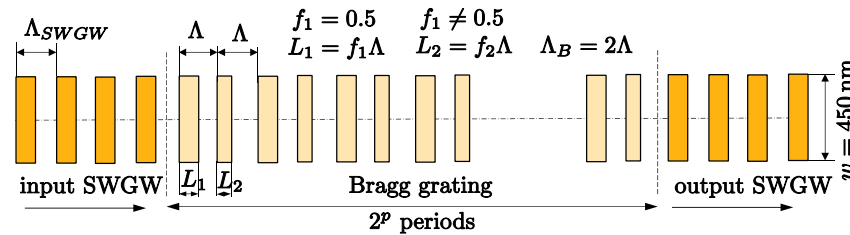


Figure 2. Schematic drawing of the SWG waveguide Bragg grating with corresponding SWG input and output waveguides.

Here, inspired with [38], our contribution is devoted to a newest special example of simulations of SWG Bragg filters [39]. As was already mentioned, the SWG waveguide supports propagation of Bloch modes. Thus, for adequate simulation (as well as for experimental characterization) of Bragg gratings, Bloch modes have to be properly excited and detected in the waveguide structure. Although experimentally, efficient SWG taper mode transformers, adiabatically transforming standard modes in silicon input and output nanowires into the Bloch modes of the SWG waveguide were proposed [36] and also theoretically analyzed in detail by us [31], for Bragg SWG filters here, we have approached them in a different way, helping save significantly both computational time and efforts. Instead of considering the influence of such tapers, we excite the SWG Bragg filters directly with the Bloch mode of the input SWG waveguide. Having calculated the scattering matrix of the Bloch modes of the structure, we could directly numerically access the corresponding reflected / transmitted optical powers. For this purpose, we have elaborated the Bloch mode calculation procedure within our RCWA/aRCWA codes, using appropriately the transformation matrices from the local normal modes to Bloch modes. In this sense, in Figure 2, a schematic picture of the analyzed Bragg grating structure in a SOI SWG waveguide is shown, with corresponding input and output SWG waveguide sections. The parameters chosen were the following: thickness of Si layer 220 nm, the width of Si segments $w = 450$ nm, in agreement with typical SWG designs; substrate and

cladding regions are made from SiO₂. Since the duty cycle of the input and output SWG waveguides is 0.5 (the same lengths of Si segments and gaps), it allows forming the Bragg grating, with the period twice as large than the standard SWG period, by adjusting the length of each second Si segment, keeping the first spacing between the segments unaffected. Modifying the Si filling factor in the second half-period of the Bragg grating (duty cycle modulation) allows its tuning, correspondingly.

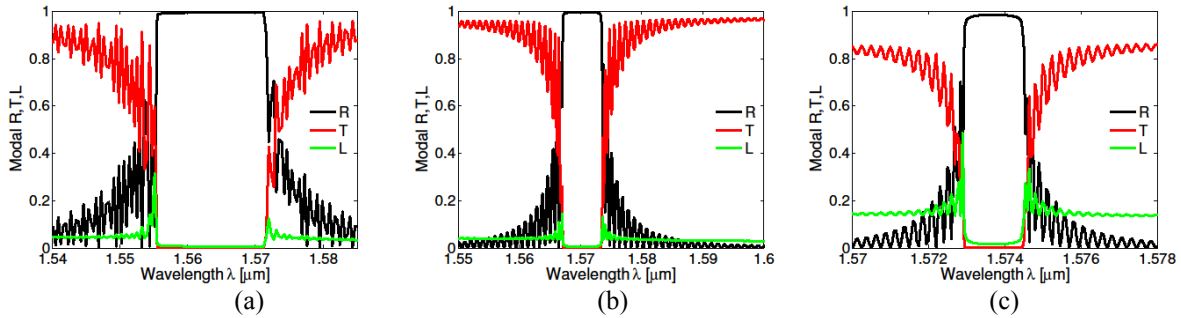


Figure 3. Calculated spectral responses of SWG Bragg gratings (modal reflectance R , transmittance T , and loss L) for the three values of the filling factor f : a) $f = 0.45$, b) $f = 0.48$, and c) $f = 0.495$. Bragg grating period $\Lambda_{\text{Bragg}} = 500$ nm, 1024 (case a, b) or 4096 (case c) periods considered, respectively.

Based on our analysis, we have found that for such computational problems, full vector 3-D tools are a necessity. An example of one of the designs is shown in Fig. 2 (Bragg grating 500 nm, SWG period 250 nm). In Fig. 3, calculated spectral characteristics corresponding to the three filling factors are shown, with 1024 or 4096 periods of the Bragg filter, respectively. While the filling factor $f = 0.45$ (Fig. 3a) gives the bandwidth over 15 nm, for $f = 0.48$ (“weaker” Bragg grating), the calculated bandwidth is still quite large (5 nm, see Fig. 3b) [39]. Even for the grating with $f = 0.495$ (4096 periods, Fig. 3c), the calculated bandwidth was still more than about 1 nm. It should be added that we have also tested the applicability of non-3D approaches finding them even more inadequate in use as in the case of simple SWG waveguides, the reason being mainly in incorrect determination of the “equivalent refractive indices of the Si void parts.

Our 3D analysis of Bragg SWG-base filters have thus confirmed, in agreement with our previous findings for simpler SWG structures, that in order to design a narrow-band filter, the critical dimensions of Bragg SWG waveguide building blocks overpass the limits of today’s fabrication possibilities. Alternative configurations (based on other types of modulation, e.g. positional one) of SWG Bragg grating designs with more relaxed requirements are hence needed.

3.2 Plasmonic Arrayed Nanostructures for Surface Plasmon Resonance Sensing

Concerning advanced plasmonic nanostructures, advanced plasmonic nanostructures with sensing potential have been of our deep interest. Our interest was directed to mapping, explaining, and finding new possibilities of effective resonant excitation of surface plasmon (SP) on such nanostructured metallo-dielectric surfaces. These structures were studied in connection to their potential in applications in SPR and / or surface enhanced Raman spectroscopy (SERS) biosensing, for the detection of chemical and biochemical species [40-43]. The dependencies of spectral positions and shapes of the resonances dips in the spectra on critical parameters were studied. Here, our RCWA technique has found its important employment. Surface plasmons, as coherent oscillations of free electrons at the boundaries between metal and dielectric, can be categorized into two classes: propagating surface plasmons (PSP) and localized surface plasmons (LSP). While PSP are propagating electromagnetic waves at an interface, in case of LSP on isolated nanostructures, there is no propagating wave at surface, but instead surface field near the particle’s surface is enhanced, due to these localized oscillations. Plasmon resonant frequencies of both PSP and LSP are highly sensitive to slight refractive index changes (caused by a change of the concentration of a measurand); this feature makes them attractive for usage in plasmonic biosensors. Clearly, both platforms, i.e. based on either PSP or LSP possess their advantaged and disadvantages. While LSP platforms typically exhibit considerably lower bulk refractive index sensitivities, the resolution corresponding to surface refractive index changes is comparable, due to higher localization of the electromagnetic field at the interface between dielectric and metal [44]. Next, we will demonstrate the effective application use of the 2D-periodic RCWA method as an efficient tool for analyzing the resonant behavior, on a specific example of a LSP-based-sensor structure based on an array of periodically arranged gold cylinders [40]. Alternatively, among other schemes, we have also studied the performance of a system of randomly spaced gold nanodisks [41]. There, we studied the optical response of Fano resonances resulting from the interference between localized surface plasmons on a random array of gold nanoparticles on a glass substrate and reflection of light at the boundary of the glass substrate. Due to a randomness of nanoparticles, we developed a new original approach enabling the treatment for such cases.

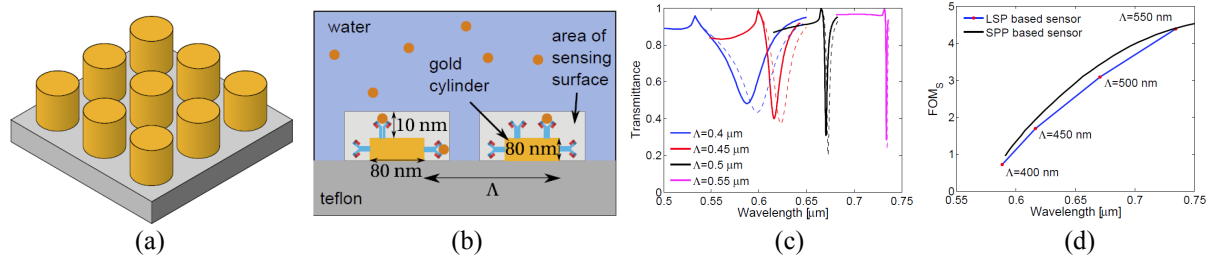


Figure 4. An example of the analyzed LSP based sensor structure based on two-dimensional periodic array of gold cylinders: a) 3D view of the sensor, b) schematic cross-sectional view, c) transmission spectra of the nanoparticle array with different periods Λ (disk radius 40 nm, disk height 80 nm, normal incidence). Dashed lines represent simulations with the surface refractive index change, d) corresponding figures of merit, red points show positions of peak minima from c).

The structure of interest is shown in Figs. 4a and 4b, together with an example of our results in terms of both transmittance (Fig. 4c) and (Fig. 4d). Due to complex physics, this structure supports combination (coupling) of LSP with Rayleigh anomaly in periodic structure (emergence of the new diffraction order (see Fig. 4a), resulting in a narrow resonance lines in spectral transmittance. Let us remind a reader that the figure of merit (FOM), characterizing a photonic aspect of the interaction, is given by the product of the surface sensitivity (related to surface refractive index changes) and a fraction, characterizing the resonant curve (height of the resonant peak over its width (typically a full width at half maximum)). The surface sensitivity defines the spectral shift of the resonance, caused by binding of an analyte, with respect to the corresponding refractive index change. In order to achieve an efficient coupling of the Rayleigh anomalies with LSP (so called surface lattice resonances), the same refractive indices of a teflon substrate and water medium are considered. Dispersion model for gold is derived either from the experimental data provided by Johnson and Christy [45], or data based on the experimental characterization of gold. As a surface refractive index change, we considered a sensing area with thickness 10 nm and refractive index 1.5. Figure 4c shows the transmission spectra at normal incidence for LSP arrays for different grating periods. The lower peaks correspond to lattice surface resonances while the upper ones correspond the Rayleigh anomalies. Dashed lines represent simulations with the appropriate surface refractive index change. Finally, Fig. 4d illustrates a comparison of FOM of the LSP based sensor under study with a standard SPP based sensor (homogeneous interface). As is seen, FOM of the LSP based sensor are comparable to that of a conventional SPP sensor. This enables its efficient usage since the surface lattice resonances allow improvements in terms of the limits of detection (given not only with the FOM, but also mass-transfer effects).

4. CONCLUSIONS

To summarize, we have presented our recent experience with all aspects of the rigorous coupled-wave analysis technique, for both periodic and aperiodic implementation. Among frequency-domain rigorous numerical methods, the RCWA/aRCWA techniques represent a quite efficient and robust tool for simulations of both periodic as well as isolated (being considered as a single period of a periodic structure) micro and nanostructures for various photonic and plasmonic applications. Recently, the importance of this approach has been even increased, as many novel designs of photonic and/or plasmonic nanostructures have been emerging, not only demonstrating new physics, but also becoming very attractive for photonic device applications. Newly, various alternative approaches / modifications to several critical parts within the algorithm have appeared; and we have also contributed to this issue, demonstrating improvements in terms of performance / time efficiency and computational capabilities. These include primarily alternatives within the correct Fourier factorization schemes and the adaptive spatial resolution techniques. Although not mentioned in this paper, we have also successfully developed and applied full anisotropic and Kerr-type nonlinear RCWA/aRCWA techniques (in 2D at the moment). As the application of our techniques, via extensive simulations, we have performed the systematic research on plethora of various novel photonic / plasmonic (nano)structures. Although new results were presented in two categories only in this paper, in last years, we have obtained novel results in a much broader portfolio of structures, ranging from advanced plasmonic guiding structures (such as novel hybrid dielectric plasmonic slot waveguides), surface plasmon resonance structures, nonlinear plasmonic couplers, 3D resonant nanostructures, plasmon-based structures with extraordinary optical transmission effects, negative-index metamaterials, and 3D synthetic opal photonic crystals. Another advantage of our methods – as in-house codes – is that they can be easily modified for novel applications not yet envisaged during their development. Recently, our calculation capabilities have also inspired new research activities in several related areas, such as the analysis of advanced substrates for surface enhanced Raman spectroscopies (SERS), special types of photonic structures with loss and gain (*PT*-symmetry breaking).

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