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REGULAR ARTICLE

Field Enhancement with Waveguide Resonance by the Structure Dielectric Grating/Dielectric Layer/Metal Substrate

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In this work, the results of modelling the diffraction of a plane wave by the structures of type dielectric grating/dielectric layer/metal substrate are presented. The strongest field enhancement is achieved for TE polarization under of waveguide mode resonance. In addition, the reflection coefficient is zero under such resonance conditions. Waveguide mode resonance can be realized in a wide range of wavelengths by changing the grating parameters. The spectral characteristics of three types of periodic structures were modelled. The first and second structures contain a dielectric layer, while the third one does not. The waveguide mode resonance and, accordingly, zero reflection coefficient can be obtained with carefully selected structure parameters. Resonant values of the grating thicknesses and periods were determined. Numerical modelling was done with Rigorous Coupled Wavelength Analysis. The thicknesses different from the resonant ones significantly affect the reflection coefficient from the periodic structure, as was established. Absolute permissible deviation values of the thicknesses of the gratings and dielectric layers from the calculated resonance values were estimated. The waveguide mode resonance is sensitive to the incident wavelength on the periodic structure. The reflection coefficient and the field distribution along the grating period were calculated. Studied structures can be effectively used as substrates for SERS-type devices due to field enhancement and zero reflection coefficient under waveguide resonance. The strongest field on the grating surface is observed for the structure without a dielectric layer, namely, dielectric grating deposited on the metal substrate. In addition, the benefits of such periodic structures include lower manufacturing costs.

Keywords: Grating, Field resonance, Waveguide mode, Metal substrate.

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1. INTRODUCTION

Raman scattering is widely used to study the vibrational spectra of molecules and optical vibrations of crystal lattices [1, 2]. The cell with the tested medium was irradiated by a light source with a narrow spectral line, preferably lasers, in particular, He-Ne with a radiation wavelength of 632.8 nm or YAG:Nd^{3+} at the second harmonic of 532 nm. The spectral lines appear as a result of the laser radiation interaction with the vibrations of molecules in the scattered light. They are shifted down in frequency by an amount equal to the vibrational frequencies of the tested medium. Such a shift in the frequency of scattered laser radiation is called the Stokes shift. In scattered light, frequencies equal to the sum of the frequencies of laser radiation and the vibrational frequencies of the tested medium are also possible. Such scattering is called anti-Stokes scattering and its power is several orders of magnitude lower than the power of Stokes scattering [3].

The simple optical scheme of the Raman spectroscopy system is shown in Fig. 1. The system consists of a Notch Filter, which does not transmit the laser radiation into the spectrometer. The scattered shift in frequency light is many orders of magnitude less powerful than the power of laser radiation reflected from the tested sample, which is not frequency-shifted. Nevertheless, the power of frequency-shifted radiation is very small, which places special demands on the spectrometer.

Surface Enhanced Raman Scattering (SERS) is often obtained with the nanostructured silver surface [4, 5] created by the electrochemical etching. Filed enhancement was achieved more than 4000 times [4]. The increase in the Raman signal is explained by the increase in the electromagnetic field on the relief silver surface due to plasmon resonance [6].

The field enhancement can be obtained not only under plasmon resonance by the silver relief surfaces but also on particles of other noble metals. Methods of field enhancement due to resonance phenomena in periodic nanostructures are well known. In particular, waveguide modes are resonant by dielectric gratings [7], resonance of surface plasmon-polariton waves by metal gratings [8], and resonance of surface plasmons [9]. The reflection coefficient can be equal to unity under waveguide resonance by dielectric gratings. It imposes some limitations on SERS systems applications.

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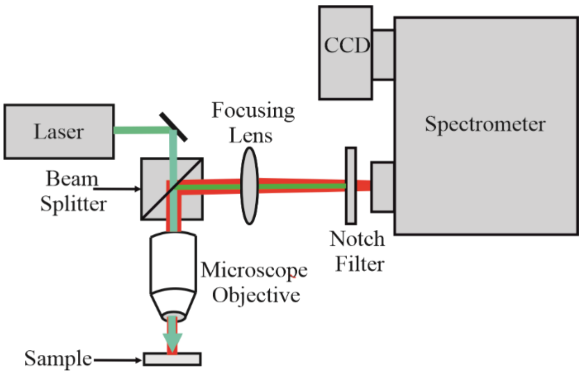

Fig. 1 – Optical scheme of the Raman spectroscopy

The waveguide modes resonance for TE and TM polarizations of incident radiation on the grating or the surface plasmon-polaritons resonance for waves of TM polarization can occur in the periodic structure of a dielectric grating on a metal surface [10]. A zero-reflection coefficient can be achieved in such a structure, thanks to the resonance of the field, with carefully selected grating parameters at the corresponding wavelengths. That is, such a structure can simultaneously be a narrow-band rejection filter in SERS systems for laser radiation not shifted in frequency. Therefore, structures of type the of dielectric grating on the metal substrate were studied as narrow-band absorbers of optical radiation, i.e. rejection filters that work based on reflection [11–13], as well as sensors for measuring changes in the refractive index of liquids and gases.

The strongest field enhancement is achieved for TE polarization waves under the waveguide modes resonance corresponding to [10]. In addition, the width of the reflection coefficient spectral response is also minimal. It should be noted that both resonances the waveguide modes and surface plasmon-polariton waves are possible for TM polarization waves. Weaker fields arise under the both resonances of the waveguide modes and the surface plasmon-polariton waves for TM polarization compared to the only waveguide modes resonance for TE polarization [10]. Therefore, it is more appropriate to use the resonance of waveguide modes for TE polarization waves in SERS systems. The usage of the waveguide mode resonance for SERS systems has an additional advantage, which is that such resonance can be realized in a wide range of wavelengths by changing the grating parameters.

Therefore, our research is aimed at improving the waveguide resonance characteristics for TE polarization waves in periodic structures of several types.

2. DESCRIPTION OF THE STUDIED STRUCTURE AND SEARCH OF RESONANT VALUES OF THE THICKNESSES AND PERIODS OF THE GRATING

The studied periodic structure is shown in Fig. 2. The dielectric grating with the thickness of d_1 is deposited on a dielectric layer with thickness of d_2. The substrate is a metal, in particular silver or gold. The various types of plasmon resonances are most clearly manifested there.

Numerical calculations were carried out for the three structures with the follow parameters:

1) $\varepsilon_{21} \neq \varepsilon_{22} \neq \varepsilon_3 = 2.25, d_1 > 0, d_2 > 0$;
2) $\varepsilon_{21} = \varepsilon_1 = 1, \varepsilon_{22} = \varepsilon_3 = 2.25, d_1 > 0, d_2 > 0$;
3) $\varepsilon_{21} = \varepsilon_1 = 1, \varepsilon_{22} = \varepsilon_3 = 2.25, d_1 > 0, d_2 = 0$.

The plane wave with wavelength of 632.8 nm is accident normal to the diffraction grating. In case of the first structure, ε_{21} and ε_{22} will be little different from each other to achieve a strong field on the grating surface [10]. It is assumed that the thickness d_1 will also be small. There is no dielectric layer in the third structure. The waveguide mode resonance and, accordingly, zero reflection coefficient can be obtained with carefully selected structure parameters.

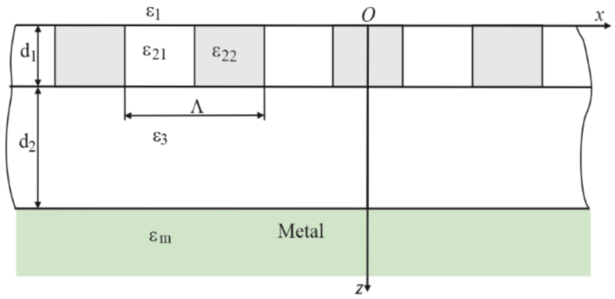

Fig. 2 – The periodic structure is a dielectric grating with a thickness of d_1 deposited on a layer of a dielectric with a thickness of d_2. Λ is the grating period. The grating filling factor is $F = 0.5$. The material of the substrate is silver with a dielectric constant of ε_m. The dielectric constant of the surrounding medium is $\varepsilon_1 = 1$ in our analysis

The grating period Λ and the thickness d_2, where $d_2 \gg d_1$ for structures of types 1 and 2, as well as d_1 for the structure of the third type, can be determined from the condition of the waveguide effect for planar waveguides based on the Ray Optics Laws [11] as follows:

$$d = 0.5\frac{\phi_1 + \phi_2 + 2\pi m}{k \sin\theta}, \quad (2.1)$$

where $\phi_1 = \arctan(\Im r_1/\Re r_1)$, $\phi_2 = \arctan(\Im r_2/\Re r_2)$, $k = 2\pi\sqrt{\varepsilon_3}/\lambda$ for 1 and 2 periodic structures and $k = 2\pi\sqrt{(1-F)\varepsilon_{21} + F\varepsilon_{22}}/\lambda$ for third periodic structure, $\theta = \arctan(k_z/k_x)$, $k_x = 2\pi/\Lambda$, $k_z = \sqrt{k^2 - k_x^2}$, $m = 0, 1, 2, \dots$, r_1 is the reflection coefficient of the waveguide mode from grating-medium (ε_1) interface, r_2 is the reflection coefficient of the waveguide mode from the metal substrate-medium (ε_3) interface.

The spectral dependences of the silver dielectric permittivity in analytical form were used from work [14] at the numerical analysis.

The dependences ϕ_1, ϕ_2 and $d = d_1 + d_2$ on the grating period for periodic structures of the first and second types are presented in Fig. 3a. The same dependences for the structure of the third type are shown in Fig. 3b. Dashed lines correspond to the exact value of $d = d_1 + d_2$. Calculations were made according to Equation (1) with $m = 1$.

Jumps in ϕ_1 and d are observed on the graphical dependences (Fig. 3). It is reasonable to assume that the resonance thicknesses and periods of the gratings are close to the jumps. The corresponding thicknesses d and grating periods are equal $d_0 = 495.4$ nm, $\Lambda_0 = 496.3$ nm for periodic structures of the first and second types and

$d_0 = 680$ nm, $\Lambda_0 = 552$ nm for structures of the third type.

Numerical modelling was done with Rigorous coupled wavelength analysis (RCWA). The reflection coefficient R from the periodic structure and the field distribution along the grating period for $z = 0$ and $z = d_1 + d_2$ were calculated. The reflection coefficient was obtained about 0.98 using the starting values of d_0 and Λ_0. However, the field amplitude at $z = 0$ was more than unity. It indicates that we are close to the resonance. In the following steps, we successively change the grating period Λ and the thicknesses d_1 and d_2. The parameters ε_{21} and ε_{22} were also changed for the periodic structure of the first type. Thus, after some corrections, the parameters of periodic structures were determined when the waveguide modes resonance occurs and the reflection coefficient from the structure is $R < 0.0001$.

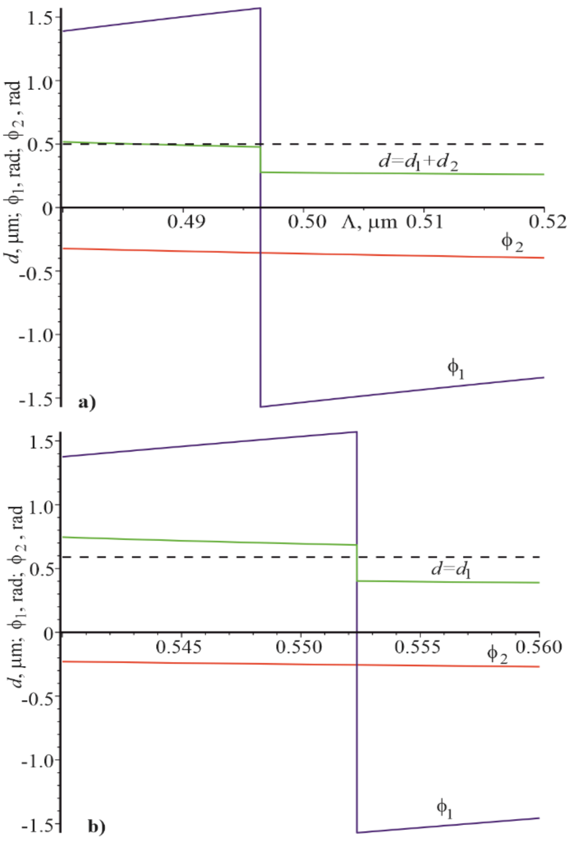

Fig. 3 – Dependences of d, ϕ_1, ϕ_2 on Λ, calculated according to equation (1): for periodic structures of the first and second types (a), and for a periodic structure of the third type (b)

Table 1 shows the starting parameters of periodic structures and the parameters when the waveguide resonance occurs.

Table 1 – Grating parameters under resonance

No	ε_{21}	ε_{22}	d_0, nm	d_1, nm	d_2, nm	Λ_0, nm	Λ, nm
1	2.4434	2.5566	495.4	100	400	496.3	444.5
2	1	2.25	495.4	11.8	471	496.3	451.4
3	1	2.25	680	592	0	552	562.3

As it can be seen from Table 1, $d_0 = 495.4$ nm is quite close to the sum of resonance values $d_1 + d_2$ for structures of the first and second types. However, Λ_0 and Λ differ much more. The difference between d_0 and d_1 is quite large, approximately 90 nm in the case of the periodic structure of the third type. The difference between Λ_0 and Λ is equal to 10.2 nm. Therefore, the approximate values of thicknesses and periods of gratings calculated with equation (1) are quite close to the resonance values. It significantly speeds up the search for resonance values of thicknesses and periods.

3. RESULTS AND DISCUSSIONS

The spectral dependences of the reflection coefficient on periodic structures of three types were calculated taking into account determined resonance thicknesses d_1 and d_2 and the period Λ of the gratings. These dependencies are shown in Fig. 4. The structure of the first type (red curve) has the lowest value of the full width at half maximum (FWHM) of the reflection spectrum. It is due to the fact that the contrast of the dielectric grating in this structure is quite low, $\varepsilon_{22} - \varepsilon_{21} = 0.1123$ at the thickness of the grating $d_1 = 100\,nm$. The third structure (blue curve) has the highest value of the FWHM spectrum. It is $\delta\lambda = 0.15$ nm, which corresponds to the spectrum width in the frequency domain $\delta v = 1.12 \times 10^{11}$ Hz. This last value should be compared with the Raman minimum frequency shift for some substances. These data can be found in the book [3]. Thus, δv is sufficiently small and equal to 519 cm^{-1} for SO_2, which corresponds to the frequency shift $\delta v = 519 \times 3 \times 10^{10} = 1.56 \times 10^{13}$ Hz. It is significantly higher by about two orders of magnitude than the width of the reflection spectrum from the periodic structure of the third type $\delta v = 1.12 \times 10^{11}$ Hz.

It should be expected that the deviation of the thicknesses d_1 and d_2 from the resonant ones can significantly affect the reflection coefficient from the periodic structure. This is due to the fact that the manifestation of the waveguide mode resonance is sensitive to the incident wavelength on the periodic structure.

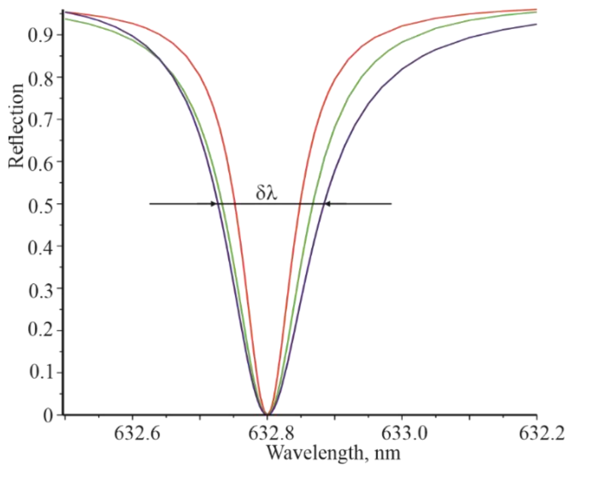

Fig. 4 – Spectral dependences of the reflection coefficient on the periodic structure at resonance parameters. The red curve represents the structure of the first type, the green curve represents the structure of the second type, and the blue one represents the structure of the third type

That is, it is necessary to determine what are the permissible deviations of d_1 and d_2 from the resonance values in order to ensure that the reflection coefficient R is less than 0.01. The corresponding dependencies are presented in Fig. 5.

It can be concluded analyzing Fig. 5a that the third structure is the most sensitive periodic structure to the relative change of d_1 (grating thickness) and the second structure is the lowest sensitive. At the same time, the sensitivity of periodic structures of the first and second type is to the relative change of d_2 (thickness of the waveguide layer) is practically the same.

It is possible to calculate the absolute permissible deviation values of the thicknesses d_1 and d_2 from the calculated resonance values using the data of Fig. 5. Thus, δd_1 for the first, second, and third periodic structures are equal to 0.025 nm, 0.1 nm, and 0.05 nm, respectively. The maximum permissible deviation δd_2 for the first and second structures is the same and equal to 0.05 nm.

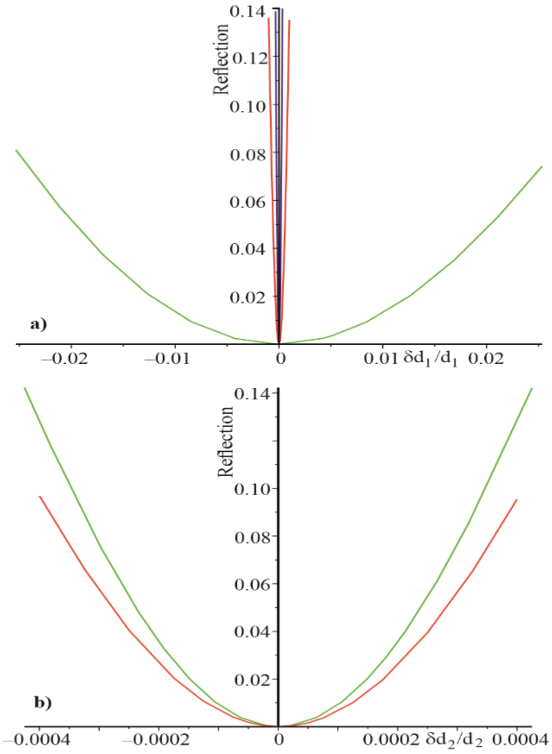

Fig. 5 – Dependences of the reflection coefficient on the relative changes in thickness d_1 (a) and d_2 (b). The red curve represents the structure of the first type, the green curve represents the structure of the second type, and the blue curve represents the structure of the third type

It should be noted that with these thickness deviations from the optimal values, the reflection coefficient increases to 0.01. The strongest field on the grating at $z = 0$ practically does not change, which is in many cases more important than the filtering properties of such structures. The field distributions along one period of the periodic structure are shown in Fig. 6.

It can be seen that the strongest field on the grating surface is observed for the third structure and the maximum value is approximately 37 relative units.

4. CONCLUSIONS

The above research results show that periodic structures of type the grating/dielectric layer/metal substrate can be used as an effective substrate for SERS-type devices due to field enhancement and zero reflection coefficient under waveguide resonance. The field on this grating surface is the strongest among all types of structures. In addition, the periodic structure of the third type is the easiest to manufacture from a technological point of view, since there is no uniform dielectric layer. If for the third periodic structure $\delta d_1 = 0.35$ nm, then the reflection coefficient from the structure will be equal to 0.31, and the field on the grating surface will decrease from 35 conditional units to 30. The inaccuracy of reproducing the grating thickness can be increased without a significant decrease on the grating surface if the filtering properties are not particularly important.

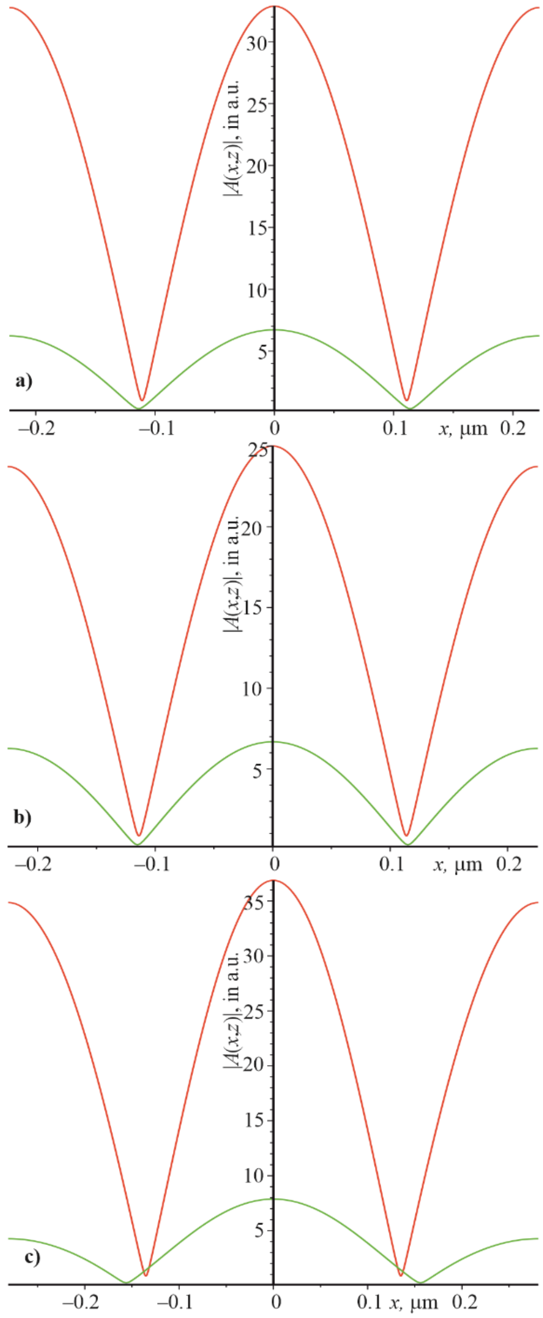

Fig. 6 – Distribution of the electric field strength modulus over one period. Red curves represent field distribution on the grating surface $z = 0$, green curves equal $z = d_1 + d_2$. Results of calculations for periodic structures of types 1, 2 and 3 are presented in (a), (b), (c) respectively

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REFERENCES

1. J. Langer, D. Jimenez de Aberasturi, J. Aizpurua, R.A. Alvarez-Puebla, B. Auguié, J.J. Baumberg, L. Liz-Marzán, *ACS Nano* **14**, 28 (2019).
2. W. Wang, P. Ma, D. Song, *Luminescence* **37**, 1822 (2022).
3. A. Yariv, *Quantum Electronics, second edition* (California Institute of Technology, John Wiley and Sons, Inc., 1975, New York London Sydney Toronto).
4. Ch.H. Lee, T. Limei, S. Singamaneni, *ACS Appl. Mater. Interfaces* **2** No 2, 3429 (2010).
5. S. Nie, S.R. Emory, *Science* **275** No 5303, 1102 (1997).
6. R. Wang, J. Ma, X. Dai, Y. Gao, C. Gu, T. Jiang. *Sensors and Actuators B: Chemical* **374**, 132782 (2023).
7. G. Quaranta, G. Basset, O.J.F. Martin, B. Gallinet, *Laser Photonics Rev.* **12**, 1800017 (2018).
8. S. Bellucci, O. Vernyhor, A. Bendziak, I. Yaremchuk, V. Fitio, Y. Bobitski, *Materials* **13** No 8, 1882 (2020).
9. Y. Zeng, R. Hu, L. Wang, D. Gu, J. He, S.Y. Wu, et al. *Nanophotonics* **6** No 5, 1017 (2017).
10. V.M. Fitio, Y.V. Bobitski, *J. Opt. A: Pure Appl. Opt.* **6** No 10, 943 (2004).
11. H.-G. Unger, *Planar Optical Waveguides and Fibres* (University Oxford, Clarendon Press, 1977, Oxford).
12. S.K. Chamoli, S.C. Singh, C. Guo, *Plasmonics*, **15**, 1339 (2020).
13. W.Z. Ma, J. Liu, G.X. Yu, W. Chen, Y.S. Chen, X.C. Deng, *Curr. Appl. Phys.* **27**, 51 (2021).
14. V. Fitio, I. Yaremchuk, O. Vernyhor, Y. Bobitski, *Optica Applicata* **50** No 2, 171 (2020).

Підсилення поля за допомогою хвилеводного резонансу структурою діелектрична ґратка/діелектричний шар/металева підкладка.

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В роботі наведено результати моделювання дифракції плоскої хвилі на структурах діелектрична ґратка/діелектричний шар/металева підкладка. Максимальне підсилення поля досягається при резонансі хвилеводних мод для TE поляризації. Крім того, коефіцієнт відбивання дорівнює нулю при резонансі хвилеводних мод для TE поляризації. Хвилеводний резонанс може бути реалізований у широкому діапазоні довжин хвиль шляхом зміни параметрів ґратки. Змодельовано спектральні характеристики трьох типів періодичних структур. Перша та друга структури містять шар діелектрика, а у третій він відсутній. Резонанс хвилеводної моди і, відповідно, нульовий коефіцієнт відбивання можна отримати за допомогою ретельно підібраних параметрів. Були визначені резонансні величини товщини і періодів ґратки. Чисельне моделювання було виконано за допомогою строгого аналізу зв'язаних довжин хвиль. Показано, що товщини, відмінні від резонансних, можуть суттєво впливати на коефіцієнт відбивання від періодичної структури. Оцінено абсолютні значення допустимого відхилення товщин ґраток і шарів діелектрика від розрахункових резонансних значень. Резонанс хвилеводних мод чутливий до довжини хвилі, що падає на періодичну структуру. Розраховано коефіцієнт відбивання та розподіл поля вздовж періоду ґратки. Досліджені структури можуть бути ефективно використані як підкладки для пристроїв типу SERS завдяки підсиленню поля та нульовому коефіцієнту відбивання при хвилеводному резонансі. Найсильніше поле на поверхні ґратки спостерігається для структури без шару діелектрика, а саме діелектричної ґратки, нанесеної на металеву підкладку. Крім того, така періодична структура найпростіша у виготовленні з технологічної точки зору.

Ключові слова: Ґратка, Резонанс поля, Хвилеводна мода, Металева підкладка.