ІНФОКОМУНІКАЦІЙНІ ТЕХНОЛОГІЇ ТА ЕЛЕКТРОННА ІНЖЕНЕРІЯ
INFORMATION AND COMMUNICATION TECHNOLOGIES, ELECTRONIC ENGINEERING

№ 5 (1), 2025

QUASI-RESONANT ABSORPTION OF TE POLARIZED WAVES BY METAL-DIELECTRIC GRATINGS

V. Fitio[ORCID: 0000-0001-6086-4087]**, D. Prokopets**[ORCID: 0009-0007-6368-4955]**, I. Yaremchuk**[ORCID: 0000-0002-7072-5950]

Lviv Polytechnic National University, S. Bandera Str., 12, 79013, Lviv, Ukraine

Corresponding author: I. Yaremchuk (e-mail: iryna.y.yaremchuk@lpnu.ua).

(Received 24 January 2025)

This paper presents a numerical study of the quasi-resonant absorption of TE-polarized waves by a periodic structure of the metal-dielectric grating type on a dielectric substrate. The parameters of such a metal-dielectric grating, in particular the period, are chosen in such a way that no waveguide resonance occurs in the grating. The absence of resonance is evidenced by low fields at grating boundaries with homogeneous dielectric media. The quasi-resonant interaction is manifested under the condition that the real part of the zeroth harmonic of the Fourier series expansion of the dielectric permittivity of the grating medium is equal to zero. This condition determines the grating filling factor which is much less than unity. The absorption, reflection, and transmission coefficients have been calculated as a function of grating thickness at the working wavelengths of 405 nm and 1064 nm. The corresponding dependences have an oscillatory character, and local absorption and transmission maxima occur at the same wavelength. The maximum of absorption, the minimum of reflection, and the maximum of transmission are observed near the wavelength of 405 nm at the grating thickness of 510 nm. It is typical of resonance phenomena in periodic structures. However, such an absorption resonance is spectrally quite broad. The fields at the grating boundaries with homogeneous dielectric media are close to the amplitude of the incident wave. The spectral characteristics of the studied structure also have an oscillatory character at the grating thickness of 625 nm and at the working wavelength of 1064 nm. Such an oscillatory character allows us to assume that the processes occurring in the studied structure are similar to the processes in the Fabry-Perot interferometer, in which there is a small absorption. Reducing the grating period leads to the decrease in the number of oscillations in the spectral characteristics. These spectral characteristics approach the spectral characteristics of the three-layer structure. Therefore, if the grating period is much less than the wavelength, then such a grating can be replaced by an equivalent multilayer structure in which metal and dielectric alternate in series. It will have approximately the same spectral characteristics.

Keywords: *grating; multilayer structure; quasi-resonance, spectral dependences; absorption; transmission and reflection*
UDC: 53.072:53:004

Introduction

Nowadays, diffraction gratings, in which the dielectric constant of the grating medium is periodically changed along a certain direction, have found wide application. In particular, gratings are used as sensitive elements of refractive index sensors. The sensors operation principle is based on resonant excitation of various waveguide processes by a periodic structure [1-5]. In such sensors, the resonance is destroyed when the refractive index changes. It is possible to restore it at a different wavelength or at a different angle of beam incidence on the grating [6,7]. Gratings are also used to field enhancement [8,9].

© 2025 Національний університет "Львівська політехніка"

This effect can be used in Raman spectroscopy to increase its sensitivity. Field enhancement can be achieved by waveguide resonance in a dielectric grating on a dielectric substrate [2,5]. Surface plasmon polariton resonance in a periodic structure of a dielectric or metal grating on a metal substrate [3,8] and surface plasmon resonance in a structure of a metal-dielectric grating on a dielectric substrate [9] can also be used. Moreover, in the latter case, the field enhancement can be several hundred times [9] at the metal-dielectric interface.

In addition, metal-dielectric gratings on the dielectric substrate with narrow dielectric gaps, the width of which is much smaller than the period, have been intensively studied. The anomalously high transmittance is achieved in such structure under certain conditions [10,11]. It is much higher than predicted by aperture theory. The transmission is achieved due to the occurrence of waveguide resonance in the grating gap [12].

Therefore, various resonances of the electromagnetic field can occur in periodic structures, which to some extents are accompanied by unexpected and non-obvious effects. For example, in the structure of a dielectric grating on a dielectric substrate under waveguide mode resonance, the reflection coefficient of the grating is equal to unity [4]. At the same time, the reflection coefficient in the structure of a metal or dielectric grating on the metal substrate can be zero under the surface plasmon polariton resonance [5].

Such a variety of effects in periodic structures prompted us to further investigate the characteristics of the interaction of a plane wave with the structure of the metal-dielectric grating on the dielectric substrate. The width of the metal part of the period was used, which is much smaller than the whole grating period and is determined by the dielectric constants. This case is interesting for TE-polarization waves, since the real part of the diagonal elements of the Toeplitz matrix in the rigorous coupled wave analysis (RCWA) equations is zero under certain conditions and the imaginary part is negligible in terms of modulus. At the same time, the elements of the matrix adjacent to the diagonal ones are quite large. That is, we have a special case, the results of the research of which are presented in this work.

2. Methods of grating diffraction analysis

The studied periodic structure is shown in Fig.1. It is a planar grating with a period Λ and a thickness d which is on the dielectric substrate with a permeability of ε_3. Part of the grating with width $F\Lambda$ is metal (Ag) with permeability ε_{22}, and the other part is dielectric with permeability ε_{21}. The spectral dependence of the dielectric constant of silver, which is presented in analytical form [13], is used for calculations. It is convenient for numerical calculations. The whole periodic structure is surrounded by the medium with ε_1. A plane wave falls normally on the grating.

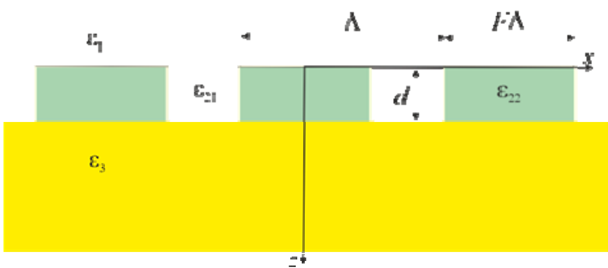

Fig.1. Schematic of the metal dielectric grating where Λ is the period of the grating, d is the thickness of the grating, F is the filling factor of the grating, which is much smaller than unity; metal is represented by the green color.

The RCWA system of linear differential equations, which describes the interaction of a TE-polarization plane electromagnetic wave with a diffraction grating, has the following form [14,15]

$$\begin{cases} \dfrac{dE_j(z)}{dz} = -ikH_j(z), \\ \dfrac{dH_j(z)}{dz} = i\dfrac{k_{j,x}^2}{k}E_j(z) - i\sum\limits_{p=-\infty}^{\infty}\varepsilon_{j-p}(z)E_p(z), \end{cases} \tag{1}$$

where r where $E_j(z)$ is the electric field strength of the coupled wave with the index j, $H_j(z)$ is the tangential component of the magnetic field strength with the index j, $k_{j,x} = k_{0,x} - j\dfrac{2\pi}{\Lambda}$, $k = \dfrac{2\pi}{\lambda}$, $k_{0,x} = \dfrac{2\pi}{\lambda}\sqrt{\varepsilon_1}\sin\theta_{1,0}$. In our case, $k_{0,x} = 0$, since the plane wave falls normally on the grating. The system of equations (1) is infinite-dimensional, but in practice a truncated system of equations is used. The number of used equations is determined by the desired accuracy of the analysis.

This system of equations (1) can be presented in matrix form and the matrix equations contain the Toeplitz matrix. The matrix elements $t_{j,p} = \varepsilon_{j-p}$ are equal to the complex coefficients of the Fourier series of the dielectric permittivity of the grating medium [14]. A rigorous mathematical justification of RCWA is given in [15]. Therefore, the diagonal elements of the Teplitz matrix are equal $t_{j,j} = \dfrac{1}{\Lambda}\int\limits_0^{\Lambda}[(1-F)\varepsilon_{21} + F\varepsilon_{22}]dx = (1-F)\varepsilon_{21} + F\varepsilon_{22}$. It means that $t_{j,j} = \overline{\varepsilon_2}$ equal to the average value of the grating medium dielectric constant.

The real part of the dielectric constant of a metal is a negative value and is much greater than unity in the modulus in the optical range for noble metals. Therefore, the real part of the diagonal elements $t_{j,j}$ will be zero at the certain value of the filling factor F determined from the formula $(1-F)\varepsilon_{21} + FR(\varepsilon_{22}) = 0$. Therefore, it can be written as follows:

$$F = \frac{\varepsilon_{21}}{\varepsilon_{21} - R(\varepsilon_{21})} \tag{2}$$

3. Results and discussion

Firstly, absorption (A), reflection (R), and transmission (T) depending on the grating thickness d at the wavelength of 405 nm were calculated by RCWA (Fig. 2). Filing factor F is equal to 0.173 at the wavelength of 405 nm with $\varepsilon_{21} = 1$ according to equation (2). In this case, the value $t_{j,j}$ is equal $t_{j,j} = +i0.0388$ and the average refractive index of the grating medium is $\overline{n_2} = \sqrt{i0.0388} = 0.139 + i0.139$. It can be seen that the average refractive index has small real and imaginary parts, which are significantly smaller units. They are also small in a narrow range of wavelengths relative to 405 nm. The corresponding dependences have an oscillatory character, and the local maxima of absorption and transmission occur at the same wavelength. In addition, the local maxima of transmission decrease and the local maxima of absorption increase as the grating thickness increases.

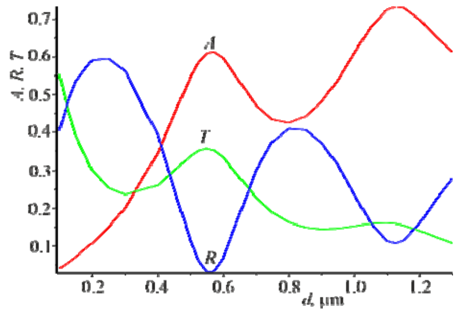

Fig.2. Dependences of reflectance (R), transmission (T), absorption (A) on the grating thickness d for $\lambda = 405$ *nm with the following parameters of the periodic structure:* $F = 0.173$, $\varepsilon_1 = \varepsilon_{21} = 1$, $\varepsilon_3 = 2.25$

The spectral dependences of *R, T* and *A* for a grating thickness of 510 nm are presented in Fig. There is a maximum in the absorption spectral characteristic near the wavelength of 405 nm. Accordingly, there is a minimum for reflection and a maximum for transmission, which is typical for resonance phenomena of periodic structures. A certain feature is present at the wavelength of 405 nm, for which $R(t_{j,j}) = 0$. However, such an absorption resonance is spectrally quite broad. The fields at the grating boundaries with homogeneous dielectric media are close to the amplitude of the incident wave. Therefore, it can be called as a quasi-resonance.

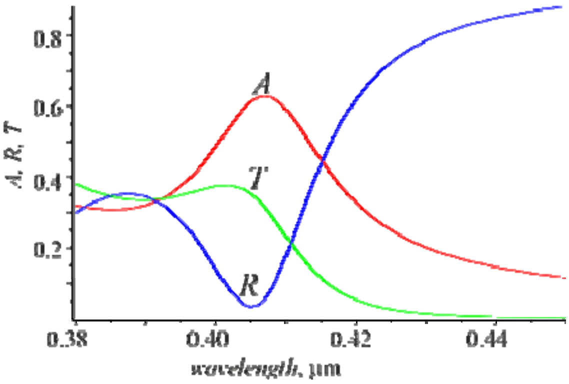

Fig.3. Spectral dependences of R, T and A at the grating thickness $d = 510$ *nm with the following grating parameters:* $\Lambda =$ *100 nm,* $F = 0.173$, $\varepsilon_1 = \varepsilon_{21} = 1$, $\varepsilon_3 = 2.25$.

The following Fig. 4 shows the dependences of *R, T* and *A* on the grating thickness for the wavelength of 1064 nm. In this case, $t_{j,j} = +i0.0468$, respectively, the average refractive index is $\overline{n_2} = \sqrt{i0.0468} = 0.153 + i0.153$. The reflection coefficient is 0.0022, transmission is 0.874, and absorption is 0.124 at the grating thickness of 625 nm. Again, there is the oscillating nature of the coefficients. This oscillatory character allows us to assume that the processes taking place in the tested structure are similar to those in the Fabry-Perot interferometer, where there is a small absorption. There are three maxima of transmittance at grating thicknesses $d_1 = 634.6$ nm, $d_2 = 1261.3$ nm, $d_3 = 1898$ nm. The thickness differences Δd between adjacent maxima will be the same and equal to 636.7 nm. This confirms the assumption that the tested structure is similar to the Fabry-Perot interferometer. The effective refractive index n_{ef} can be entered for the grating medium. The real part of which can be determined from the equation as follows:

$$\frac{2\pi R(n_{ef})d}{\lambda} = m\pi, \tag{3}$$

where m is whole number.

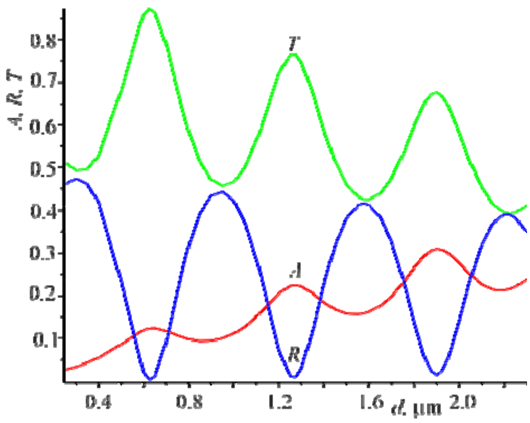

Fig.4. Dependence of reflection (R), transmission (T), absorption (A) on the grating thickness d for $\lambda = 1064$nm with the following grating parameters: $\Lambda = 264$ nm, $F = 0.0366$, $\varepsilon_1 = \varepsilon_3 = 4, \varepsilon_{21} = 2.25$

We can find $R(n_{ef}) = \dfrac{\lambda}{2\Delta d}$ based on equation (3). In our case, $R(n_{ef}) = 0.836$, which is significantly greater than $R(\bar{n}_2) = 0.153$. This increase in n_{ef} of the grating medium can be explained by the fact that part of the photons propagates in the grating medium as in a waveguide due to diffraction in the ± 1st order. As a result, photons in the grating are delayed for a time that is longer than the time for the normal propagation of a photon through the grating, which leads to an increase in n_{ef}.

The spectral characteristics for a grating thickness of 1900 nm are showed in Fig. 5. The nature of these curves confirms the previous conclusion regarding the Fabry-Perot interferometer. A slight deviation from the condition $(1-F)\varepsilon_{21} + FR(\varepsilon_{22}) = 0$ will appear as the wavelength changes, since F is constant for all wavelengths, and ε_{22} depends on the wavelength.

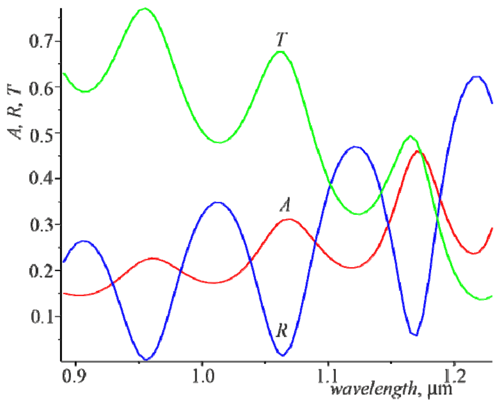

Fig.5. Dependence of reflection (R), transmission (T), absorption (A) on the grating thickness $d = 1900$ nm for the following grating parameters: $\Lambda = 264$ nm, $F = 0.0366$, $\varepsilon_1 = \varepsilon_3 = 4, \varepsilon_{21} = 2.25$

The spectral dependences of R, T and A with slightly different parameters of the periodic structure near the wavelength of 405 nm are showed in Fig. 6. Again, there is the oscillatory nature of the spectral dependences. However, these dependencies are changed slightly compared to Fig. 3 due to changes in ε_1 and ε_{21}, which leads to the change in the filling factor F.

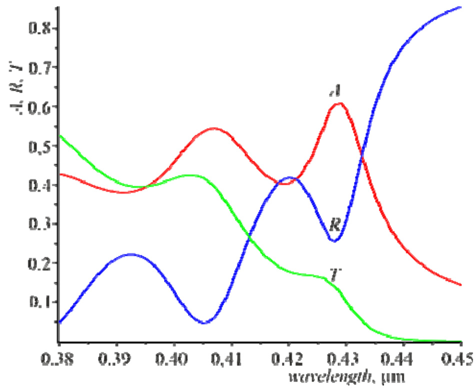

Fig.6. Dependence of reflection (R), transmission (T), absorption (A) on wavelength for the following grating parameters:

$\Lambda = 100\ nm,\ d = 625\ nm,\ F = 0.321,\ \varepsilon_1 = \varepsilon_3 = \varepsilon_{21} = 2.25$

The spectral dependencies change qualitatively when the grating period is reduced, such as 10 nm. These R and T dependencies are shown in Fig. 7. The continuous curve represents the equivalent three-layer structure homogeneous along the x coordinate for $= 625$ nm, $\varepsilon_1 = \varepsilon_3 = 2.25$, $\varepsilon_2 = \varepsilon_{21}(1-F) + \varepsilon_{22}F$. Filled rings represent the grating with a period $\Lambda = 10nm$. Rings represent the equivalent multilayer structure with the number of layer pairs of $N = 40$, which is shown in Fig. 8. In this case the thickness of the dielectric nanolayer with ε_{21} is equal to $d(1-F)/N$ and the thickness of the metal nanolayer is dF/N.

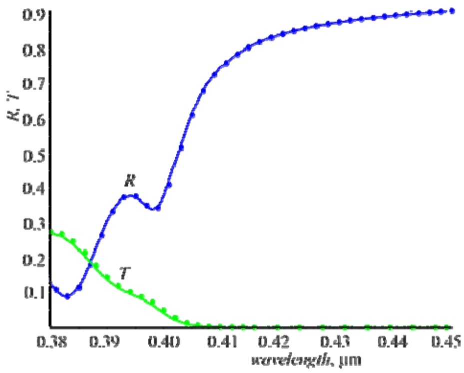

Fig.7. Spectral dependences of R and T for three different structures, for calculations it is assumed that $F = 0.321$.

As the grating period decreases, the number of oscillations in the spectral characteristics decreases, as shown in Fig. 7. These spectral characteristics become the spectral characteristics of the three-layer structure with a dielectric constant $\varepsilon = \varepsilon_{21}(1-F) + \varepsilon_{22}F$. In this case, $\varepsilon = i0.0717$, which is practically impossible to realize in the form of a single homogeneous layer. Such an equivalent value of ε can be achieved by using a large number of pairs of dielectric and metal nanolayers. Such a structure is shown in Fig. 8.

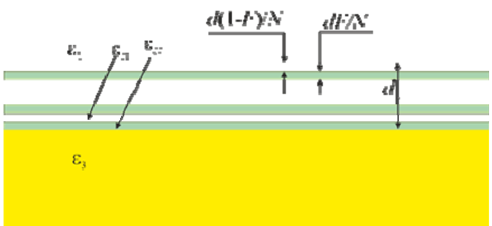

Fig.8. An equivalent multilayer pattern with a spectrum that closely resembles a 10-nm periodic pattern.

Conclusion

A study of the periodic structure of the metal-dielectric grating on the dielectric substrate at the filling factor F where the real part of the average dielectric constant of the grating medium is zero at certain wavelengths (405 nm and 1064 nm), has been carried out. The dependencies of transmission and reflection on wavelength and grating thickness for the grating period of 100 nm have an oscillatory character. Moreover, these dependencies are similar to those of a Fabry-Perot interferometer, in which the effective part of the effective refractive index of the grating medium $R(n_{ef})$ is significantly higher than $R(\bar{n}_2)$. Such an increase in n_{ef} of the grating medium can be explained by the fact that photons are delayed by the time due to diffraction. This time is greater than the time for normal photon propagation through the grating.

The grating can be replaced by an equivalent multilayer structure with periodic alternation of metal and dielectric when the grating period is much smaller than the wavelength, in particular 10 nm. The number of layer pairs should be large enough, in our case 40 pairs.

Acknowledgment

This research was funded by the Ministry of Education and Science of Ukraine and should be acknowledged ("Development of plasmonic nanostructured substrates for SERS signal enhancement in the detection of explosives", 0124U000823).

References

[1]. Xu, Y., Bai, P., Zhou, X., Akimov, Y., Eng Png, C., Ang, L.-K., Knoll, W., Wu, Lin. "Optical Refractive Index Sensors with Plasmonic and Photonic Structures: Promising and Inconvenient Truth". In Advanced Optical Materials, Vol. 7, pp.1801433(47), 2019, https://doi.org/10.1002/adom.201801433

[2]. Quaranta, G., Basset, G., Martin, O. J., & Gallinet, B. "Recent advances in resonant waveguide gratings». IN Laser & Photonics Reviews, Vol. 12, No 9, 1800017, 2018, https://doi.org/10.1002/lpor.201800017

[3]. Homola, J. "Surface plasmon resonance sensors for detection of chemical and biological species". In Chemical reviews, Vol. 108, No 2, pp. 462-493, pp. 2008, https://doi.org/10.1021/cr068107d

[4]. Wang, S. S., & Magnusson, R. J. A. O. "Theory and applications of guided-mode resonance filters". In Applied optics, Vol. 32, No 14, pp. 2606-2613, 1993, https://doi.org/10.1364/AO.32.002606

[5]. Bellucci, S., Fitio, V., Yaremchuk, I., Vernyhor, O., Bendziak, A., & Bobitski, Y. "Comparison of the optical planar waveguide sensors' characteristics based on guided-mode resonance". In Symmetry, Vol. 12, No 8, pp. 1315, 2020, https://doi.org/10.3390/sym12081315

[6]. Puiu, M., & Bala, C. "SPR and SPR imaging: recent trends in developing nanodevices for detection and real-time monitoring of biomolecular events". In Sensors, Vol. 16, No 6, pp. 870, 2016, https://doi.org/10.3390/s16060870

[7]. Yoon, K. H., Shuler, M. L., & Kim, S. J. "Design optimization of nano-grating surface plasmon resonance sensors". In Optics express, Vol. 14, No 11, pp. 4842-4849, 2006, https://doi.org/10.1364/OE.14.004842

[8]. Bellucci, S., Vernyhor, O., Bendziak, A., Yaremchuk, I., Fitio, V. M., & Bobitski, Y. "Characteristics of the Surface Plasmon–Polariton Resonance in a Metal Grating, as a Sensitive Element of Refractive Index Change". In Materials, Vol. 13, No 8, pp. 1882, 2020, https://doi.org/10.3390/ma13081882

[9]. Fitio, V., Yaremchuk, I., Vernyhor, O., & Bobitski, Y. "Resonance of surface-localized plasmons in a system of periodically arranged gold and silver nanowires on a dielectric substrate". In Applied Nanoscience, Vol. 8, pp. 1015-1024, 2018, https://doi.org/10.1007/s13204-018-0686-z

[10]. Popov, E., Neviere, M., Enoch, S., & Reinisch, R. "Theory of light transmission through subwavelength periodic hole arrays". In Physical Review B, Vol. 62, No 23, pp. 16100, 2000, https://doi.org/10.1103/PhysRevB.62.16100

[11]. Treacy, M. M. J. "Dynamical diffraction explanation of the anomalous transmission of light through metallic gratings". In Physical Review B, Vol. 66, No 19, pp. 195105, 2002, https://doi.org/10.1103/PhysRevB.66.195105

[12]. Cao, Q., & Lalanne, P. "Negative role of surface plasmons in the transmission of metallic gratings with very narrow slits". In Physical Review Letters, Vol. 88, No 5, pp. 057403, 2002, https://doi.org/10.1103/PhysRevLett.88.057403

[13]. Fitio, V., Yaremchuk, I., Vernyhor, O., & Bobitski, Y. "Analytical expressions for spectral dependences of silver, gold, copper and aluminum dielectric permittivity". In Optica Applicata, Vol. 50, No 2, pp. 171-184, 2020, DOI: 10.37190/oa200201

[14]. Moharam, M. G., Grann, E. B., Pommet, D. A., & Gaylord, T. K. "Formulation for stable and efficient implementation of the rigorous coupled-wave analysis of binary gratings". JOSA a, Vol. 12, No 5, pp. 1068-1076, 1995, https://doi.org/10.1364/JOSAA.12.001068

[15]. Civiletti, B. J., Lakhtakia, A., & Monk, P. B. "Analysis of the rigorous coupled wave approach for s-polarized light in gratings". Journal of Computational and Applied Mathematics, Vol. 368, pp. 112478, 2020, https://doi.org/10.1016/j.cam.2019.112478

[16]. Dobrowolski, J. A. Optical properties of films and coatings. Handbook of Optics I, 42-3, 1995.

КВАЗІРЕЗОНАНСНЕ ПОГЛИНАННЯ ТЕ ПОЛЯРИЗОВАНИХ ХВИЛЬ МЕТАЛО-ДІЕЛЕКТРИЧНИМИ ҐРАТКАМИ

Володимир Фітьо, Дмитро Прокопець, Ірина Яремчук

Національний університет «Львівська політехніка» вул. С. Бандери, 12, 79013, Львів, Україна

У роботі проведено чисельне дослідження квазірезонансного поглинання ТЕ-поляризованих хвиль періодичною структурою типу металева гратка заповнена діелектриком на діелектричній підкладці. Параметри такої метало-діелектричної гратки, зокрема період, підібрані такими, щоб не виникав хвилеводний резонанс у ґратці. Про відсутність резонансу свідчать низькі поля на межах ґратки з однорідними діелектричними середовищами. Квазірезонансна взаємодія проявляється при умові, якщо реальна частина нульової гармоніки розкладу діелектричної проникності середовища ґратки в ряд Фур'є рівна нулю. З цієї умови визначається коефіцієнт заповнення ґратки, який набагато менший одиниці. Розраховано коефіцієнти поглинання, відбивання та пропускання в залежності від товщини ґратки для робочих довжин хвилі 405 нм та 1064 нм. Відповідні залежності мають осцилюючий характер і локальні максимуми поглинання та пропускання відбуваються на одній довжині хвилі. Для товщини ґратки 510 нм, поблизу довжини хвилі 405 нм на спектральній характеристиці поглинання спостерігається максимум, відповідно мінімум для відбивання і максимум для пропускання, що є типовим для резонансних явищ в періодичних структурах. Проте такий резонанс поглинання є спектрально досить широким, а поля на межах ґратки з однорідними діелектричними середовищами є близькими до амплітуди падаючої хвилі. При товщині ґратки 625 нм на робочій довжині хвилі 1064 нм спектральні характеристики досліджуваної структури також мають осцилюючий характер. Це дозволяє зробити припущення, що процеси, які проходять в досліджуваній структурі подібні до процесів в інтерферометрі Фабрі-Перо, у якому присутнє невелике поглинання. Зменшення періоду ґратки приводить до зменшення кількості осциляцій на спектральних характеристиках, а самі спектральні характеристики прямують до спектральних характеристик тришарової структури. Отже, якщо період ґратки набагато менший довжини хвилі, то таку ґратку можна замінити еквівалентною багатошаровою структурою, в якій послідовно чергуються метал і діелектрик і яка матиме приблизно ті самі спектральні характеристики.

Ключові слова: *гратка; багатошарова структура; квазірезонанс, спектральні залежності; поглинання; пропускання та відбивання*