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REGULAR ARTICLE

Oblique Incidence *E*-polarized Photons on Infinite Periodic Grating of Metal Strips

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Diffraction of a homogeneous unit density flow of E-polarized photons on a grating of infinitely thin metallic strips is considered. Probability of finding a photon in any point is represented by psi-function, satisfying to Schrödinger equation and boundary conditions of equality zero on the strips and continuity on the slits. This work provides further development of quantum-mechanical contemplation of the diffraction problem on the periodical structures. To solve the problem, the strict Riemann-Hilbert boundary value problem method is used. The essence of it is that the solution of the functional equations system is reduced to the restoration of the analytical function in the entire plane of the complex variable, based on the sum of its limit values on the arc of the unit circle. The unknown coefficients of the function, represented as a Fourier series, are determined from a well-converging infinite system of algebraic equations.

Using PC, numerical experiments were performed to study the probability distribution of *E*-polarized photons with a wide change in the parameters of the problem. The dependences of the square of the psi-function module on the ratio between the wavelength and the grating period, on the ratio between the slit width and the grating period are presented for different values of the angle of incidence of the photon flux and the distance from the grating. Based on the analysis of the obtained dependencies, conclusions about the ratios of parameters at which the grating constant can be determined more accurately from the observed diffraction pattern were made. With normal incidence on the grating, it is more convenient to do this by observing the diffraction pattern behind the grating, with oblique incidence - in front of the grating.

Keywords: Diffraction, Grating, Quantum, Psi-Function, Probability amplitude, Diffraction pattern, Photon.

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1. INTRODUCTION

This work provides further development and quantum mechanical contemplation to the solution of the diffraction problems on the periodical structures. To solve the problem, the strict Riemann-Hilbert boundary value problem method is used. The essence of it is that the solution of the functional equations system is reduced to the restoration of the analytical function in the entire plane of the complex variable, based on the sum of its limit values on the arc of the unit circle. The unknown coefficients of the function, represented as a Fourier series, are determined from a well-converging infinite system of algebraic equations.

The system equations are fit for any relations between wavelength and period of the structure and any relations between a width of slit and a width of a strip. Good convergence of the system permits to utilize reduction method, what make its convenient for numerical calculations with help of PC.

2. FORMULATION OF PROBLEM

Let a homogeneous unit density flow of E-polarized photons falls from the negative side of the OZ axis on a grating of infinitely thin metallic strips. Velocity of photons lies in the plane YOZ and made an angle with axis OZ. Width of slit equals d, period of grating – l, so the width of strip equals l-d (see Fig. 1).

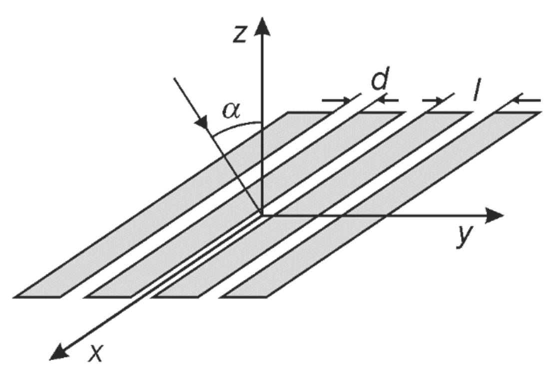

Fig. 1 – Diffraction grating

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It is needed to define intensity of flux (the probability $|\Psi|^2$ of photons above and under grating. According to de-Broglie [1] Ψ- function may be presented as

$$\Psi_0 = \exp[-\frac{i}{\hbar}(E - \vec{p}\vec{r})] \tag{1}$$

where E – energy, p – pulse of photon.

Let us consider stationary happening, then

$$\Psi_0 = \exp[i\frac{p}{\hbar}(y\sin\alpha - z\cos\alpha)] \tag{2}$$

Due to the periodicity of the structure in the direction of the Y axis, the psi-function of reflected photon can be represented as a Fourier series

$$\Psi^r = \sum_{n=-\infty}^{\infty} a_n \exp[i(\chi_n z + \zeta_n y)] \tag{3}$$

For a photon that has passed through the grating, we will have, respectively,

$$\Psi^t = \sum_{n=-\infty}^{\infty} b_n \exp[i(-\chi_n z + \zeta_n y)] \tag{4}$$

where

$$\begin{gathered}\zeta_n = \frac{2\pi n}{l} + \frac{p}{\hbar}\sin\alpha = \frac{2\pi n}{l}(1 + \frac{\vartheta}{n}\sin\alpha) \\ \chi_n = \sqrt{\frac{p^2}{\hbar^2} - \zeta_n{}^2} = \frac{2\pi|n|}{l}\sqrt{\frac{\vartheta^2}{n^2} - (1 + \frac{\vartheta}{n}\sin\alpha)}, \quad \vartheta = \frac{l}{\lambda}\end{gathered} \tag{5}$$

The total amplitude describing the state of a photon in the upper half-plane is equal to the sum of the probability amplitudes (2) and (4)

$$\Psi = \Psi_0 + \Psi_r \tag{6}$$

It must mark, that at the oblique incidence of pho-tons on a grating a vector character Ψ-function manifests itself which, by the way, Vakarchuk mentions in his book [1]. It's naturally, because Ψ -function deter-mines the state of a photon, which has electromagnetic nature and its state, is determined by strength electric and magnetic field vectors. Let us resume, that metal strips have ideal conductivity and photons cannot penetrate into metal strips. Consequently, on the strips the psi-function should vanish, and on the slits the psi-function and its derivatives should be continuous. For E-polarized photon it will be different from zero components electromagnetic field E_x,

$$H_y = -\frac{i}{k}\frac{\partial Ex}{\partial z}, \quad H_y = \frac{i}{k}\frac{\partial Ex}{\partial y}$$

It is worth noting the peculiarity of the representation of psi-functions (3), (4). Unlike the normal incidence of photons on the grating, where the psi-function is a periodic function with a period of l, psi-functions (3), (4) are almost periodic functions of the Y coordinate. But even in this case $|\Psi|^2$will represent the intensity of the photon flux above ($z \le 0$) and under ($z \ge 0$) of a grating.

On slits $\frac{\partial\Psi}{\partial y}$ and $\frac{\partial\Psi}{\partial z}$ are continuous. Satisfying the continuity condition we obtain the equality.

$$1 + \sum_{n=-\infty}^{\infty} a_n\chi_n \exp(i\frac{2\pi n}{l}y) = \sum_{n=-\infty}^{\infty} b_n\chi_n \exp(i\frac{2\pi n}{l}y) \tag{7}$$

Thus, the psi-function is continuous over the entire period. From this follow the equalities

$$b_0 = 1 + a_0, \quad b_n = a_n \tag{8}$$

Let us introduce the smallest parameter. Let's write χ_n in the form

$$\chi_n = i|n + \vartheta\sin\alpha|(1 - \eta_n) \tag{9}$$

where

$$\eta_n = 1 + i\sqrt{\frac{\vartheta^2}{(n + \vartheta\sin\alpha)^2} - 1} \tag{10}$$

tends to zero when $|n| \to \infty$. For the unknown's b_n, a_n we get the system of equations

$$\sum_{n=-\infty}^{\infty} b_n \exp(i\frac{2\pi n}{l}y) = 0, \ \text{(strip)} \tag{11}$$

$$\sum_{n=-\infty}^{\infty} b_n |n - \vartheta\sin\alpha|(1 - \eta_n)\exp(i\frac{2\pi n}{l}y) = 0, \ \text{(slit)} \tag{12}$$

We will not give mathematical explanations of the procedure for reducing of system of equations (11), (12) to a standard form, which allows writing down the solution of the Riemann-Hilbert boundary value problem. They are described in sufficient details in the monograph [2]. Finally, we have an infinite convergent sys-tem of linear algebraic equations that allows the application of the reduction method.

$$\begin{gathered}x_m = -i\vartheta\cos\alpha V_m^0 + 2\sum_{n=0}^{\nu} x_n V_m^n + \\ + \sum_{n=-\infty}^{\infty} x_n \frac{|n + \vartheta\sin\alpha|}{n + \vartheta\sin\alpha}\eta_n e^{in\phi} + 2CR_m\end{gathered} \tag{13}$$

$$\begin{gathered}0 = -i\vartheta\cos\alpha V_\sigma^{01} + 2\sum_{n=0}^{\nu} x_n V_\sigma^{n1} + \\ + \sum_{n=-\infty}^{\infty} x_n \frac{|n + \vartheta\sin\alpha|}{n + \vartheta\sin\alpha}\eta_n V_\sigma^{n1} + 2CR_\sigma^1\end{gathered} \tag{14}$$

$$(m = 0, \pm1, \pm2, \pm3, \ldots)$$

where $\varphi = 2\pi y/1$, ν - integer, satisfying the relations $\upsilon + \vartheta\sin\alpha < 0, \upsilon + 1 + \vartheta\sin\alpha > 0$.

Expressions of coefficients V_o^{ol}, V_σ^o, V_σ^n, V_m^o, V_m^n, R_σ^l, R_m in Legendry's polynomials are represented also in the work [2]. Thanks to the parameter χ_n, which tends to 0 as $\chi_n =$

$0(1/n^2)$ at $n \to \infty$ the system (9) is convergent and let to applied the reduction method

3. ANALYSIS OF OBTAINED RESULTS

When a homogeneous, monochromatic photon flux falls at an angle to the normal to the plane of the grating, a discrete spectrum of directions is formed along which the reflected and transmitted photons propagate at disc reangles to the normal. Since we assume that the frequency of the photons remains unchanged, their energy and module of momentum remain unchanged. According to (3), (4), the y-component of the photon momentum can acquire with a certain probability an increment $\Delta p_y = 2\pi n\hbar/1$, ($n = 0, \pm1, \pm2, \pm3, \ldots$). It leads to a change in the direction of its movement.

The angles at which photons can propagate are determined from the relation

$$\sin\theta_n = \frac{p_y}{p} = \sin\alpha + n\frac{\lambda}{l} \qquad (15)$$

where ($n = 0, \pm1, \pm2, \pm3, \ldots$). $p = 2\pi\hbar/\lambda$ - total moment of photon.

The basic equation of the diffraction grating (15) determines the directions of diffracted photons in the diffraction orders. It is of a universal nature and does not depend on the profile of the grating.

At $\alpha = 0$ it goes over to the equation of the diffraction grating known from wave optics

$$\sin\theta_n = n\frac{\lambda}{l} \qquad (16)$$

It should be noted, that at a normal incidence the threshold value of the ratio, determining the appearance of the diffraction patterns, as we see, depends only on the ratio between the wavelength and the period of the structure [3]. At oblique incidence it also becomes dependent on the angle of incidence and is determined by the expression

$$l/\lambda = \frac{1}{1-\sin\alpha} \qquad (17)$$

Now let us pass to discussion of numerical results. Calculations were performed using a computer program that allows to obtain the dependence the diffraction pattern on ratio period of a grating to wavelength $\vartheta = 1/\lambda$, coefficient of fulfill d/l at the different angles incidents, and at the different distances from a grating.

Putting in the system of equations (13), (14) $\chi_n = 0$ for all n, $n > N$, $-\nu > n$ and it is possible to get the limiting system. Computer program permits to do calculation in the limits of d/l from 0 to 1, and in the limits of $\vartheta = 1/\lambda$ from 0 to 4.1. Psi-function of a photon passed throw a grating or reflected is represented by expres-sion (3), (4). At the distance from plane of grating $z > l$ in the sum (3), (4), will be only the members of a number for which $n > N$, $-\nu > n$.

$$\Psi^r = \sum_{n=-\nu}^{N} a_n \exp[i(\chi_n z + \zeta_n y)] \qquad (18)$$

$$\Psi^t = \sum_{n=-\nu}^{N} a_n \exp[i(-\chi_n z + \zeta_n y)] \qquad (19)$$

Fig. 2 shows the dependences on y/l at normal incidence for different values of z/l, separated from each other by a distance of $\Delta\frac{z}{l} = 0{,}3775$ – a quarter of the repetition period of the diffraction pattern. From a comparison of the curves, it is evident that when the distance changes by the value $\Delta\frac{z}{l} = 0{,}755$ of the maximum moves from the middle of the slit to the middle of the tape and through the distance $\Delta\frac{z}{l} = 1{,}55$ is repeated.

The pattern is symmetrical both relative to the middle of the slit and the middle of the tape, which follows from the relations

$$a_n = a_{-n}, \quad b_n = b_{-n} \qquad (20)$$

that is, the psi-function is an even function with respect to the variable *y*.

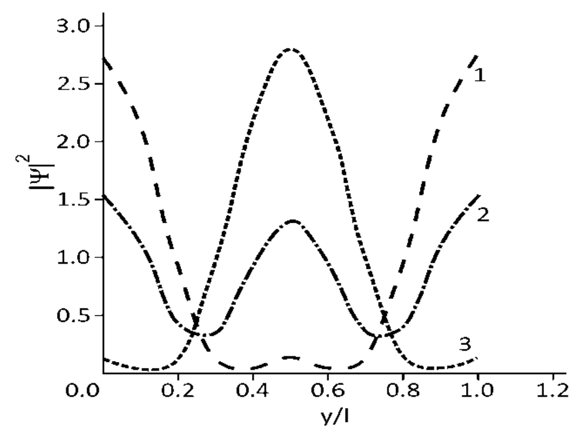

Fig. 2 – Diffraction patterns of distribution of $|\Psi|^2$ from y/l at $l/\lambda = 1.1$, $d/l = 0{,}5$, $\alpha = 0$ for different values of z/l: 1. $z/l = 1{,}55$; 2. $z/l = 1.925$; 3. $z/l = 2{,}3$

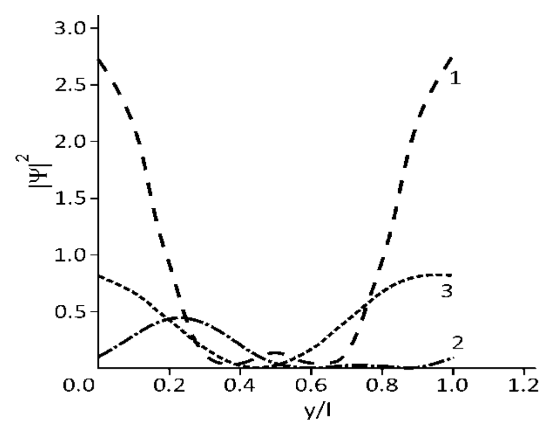

Fig. 3 – Dependence of $|\Psi|^2$ from y/l at $l/\lambda = 1.1$, $d/l = 0{,}5$, $z/l = 1{,}55$ for different values of the incidence angles: 1. $\alpha = 0$; 2. $\alpha = \pi/6$; 3. $\alpha = \pi/3$

As can be seen from Fig. 3, in the case of oblique incidence, the symmetry of the diffraction pattern is violated and violation increases with increasing of angle of incidence. This is due to the fact, that at oblique incidence, relation (20) is not satisfied. On the other hand, this is also due to the fact that new angles at which photons can propagate for negative values of n appear at smaller values of the ratio l/λ than for positive n. For the reflected photon flux, the diffraction pattern has the same character as for the transmitted one, it also repeats depending on the distance. Fig. 4 shows a family of curves for photons passed through the grating for different wavelengths.

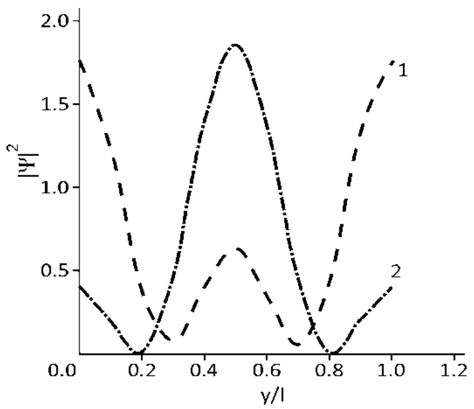

Fig. 4 – Dependence of $|\Psi|^2$ from y/l at $l/\lambda = 2.5$, $d/l = 0,5$, $\alpha = 0$ for different values of the z/l: 1. $z/l = 1,55$; 2. $z/l = 1,075$

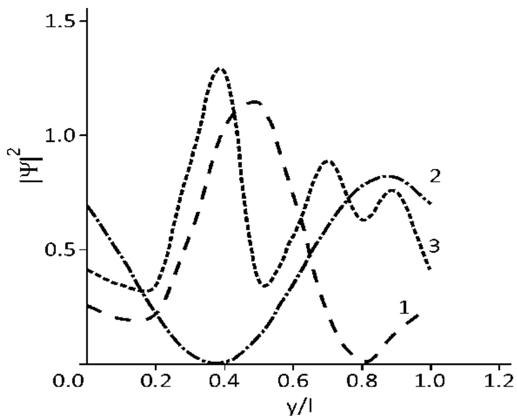

Fig. 5 – Dependence of $|\Psi|^2$ from y/l at $\alpha = \pi/6$, $d/l = 0,5$, $z/l = 3,1$ for different values of l/λ: 1. $l/\lambda = 1,1$; 2. $l/\lambda = 1,7$; 3. $l/\lambda = 2,4$

As can be seen from the graphs, with an increase in l/λ, the number of maxima increases, the diffraction pattern becomes more complicated. From the general analysis of the obtained graphs, we can draw conclusions about the values l/λ and angles of incidence at which it is more convenient to determine the lattice period from the diffraction pattern. If we satisfy the conditions $\lambda > c$ (where c is the constant of the crystal lattice in the direction of the X axis), then in this direction the photons of the atoms will perceive it as a continuous band and at the same time, will satisfy the relation

$$\frac{2}{2-\sin\alpha} > l/\lambda > \frac{1}{1-\sin\alpha} \qquad (21)$$

Then in the transmitted and reflected flows only two directions will be realized and in the diffraction pattern one clearly expressed maximum will be observed (Fig. 4) repeating with a period l. Thus, knowing the wavelength, one can determine the lattice constant.

4. CONCLUSION

1. Diffraction of a homogeneous unit density flow of E-polarized photons on a grating of infinitely thin metallic strips is considered. To solve the problem, the strict Riemann-Hilbert boundary value problem method is used. The dependences of the square of the psi-function module on the ratio between the wavelength and the grating period, on the ratio between the slit width and the grating period are presented for different values of the angle of incidence of the photon flux and the distance from the grating.

2. Periodic changes in the diffraction pattern with a change in the distance from the grating are determined. An expression is established that gives the dependence of the threshold value of diffraction, the ratio between the period of the structure and the wavelength, and on the angle of incidence. Recommendations are given regarding the ratio between the grating period and the wavelength at which either the wavelength should be measured when the period is known, or the grating constant when the wavelength is known.

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Похиле падіння *E*-поляризованих фотонів на нескінченну періодичну ґратку металевих стрічок

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Розглянуто дифракцію однорідного потоку одиничної густини Е-поляризованих фотонів на решітці нескінченно тонких металевих смуг. Імовірність знаходження фотона в будь-якій точці представлена псі-функцією, що задовольняє рівнянню Шредінгера і граничним умовам рівності нулю на смугах і неперервності на щілинах. Ця робота передбачає подальший розвиток квантовомеханічного підходу до розв'язання задач дифракції на періодичних структурах. Для вирішення задачі використовується строгий метод крайової задачі Рімана-Гільберта. Суть його полягає в тому, що розв'язок системи функціональних рівнянь зводиться до відновлення аналітичної функції у всій площині комплексної змінної за сумою її граничних значень на дузі одиничного кола. Невідомі коефіцієнти функції, представлені у вигляді ряду Фур'є, визначаються із нескінченної системи алгебраїчних рівнянь, що добре сходиться.

За допомогою ПК проведено чисельні експерименти з дослідження розподілу ймовірностей Е-поляризованих фотонів із широкою зміною параметрів задачі. Наведено залежності квадрата модуля псі-функції від відношення довжини хвилі до періоду ґратки, від відношення ширини щілини до періоду ґратки для різних значень кута падіння потоку фотонів і відстані від ґратки. Оскільки графічні залежності періодично повторюються, вони подані для одного періоду. На основі аналізу отриманих залежностей зроблено висновки щодо співвідношення параметрів, при яких за спостережуваною дифракційною картиною можна точно визначити сталу ґратки. При нормальному падінні на ґратку це зручніше робити, спостерігаючи дифракційну картину за ґраткою, при похилому падінні - перед ґраткою.

Ключові слова: Дифракція, Решітка, Квант, Псі-Функція, Амплітуда ймовірності, Дифракційна картина, Фотон.