УДК 535.4 PACS: 42. 25. Dd.42.25Hz

# Research of altitude of potential barrier at the metal-vacuum interface by the diffraction method

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The paper considers the problem of diffraction at normal incidence of a monochromatic beam of photons on a grating of thin metal strips. Quantum-mechanical approach is used to describe the phenomenon of diffraction of particles. Based on the elastic interaction of photons with electrons, that is in the strip and carries a one-dimensional movement in the potential pit with barriers of finite height, relations for discrete values of angles, at which the diffraction peaks should be observed, were obtained in the first approximation. The equations obtained in this work are the same in the case of small angles of diffraction as the known in the scientific literature expressions that determine the position of the diffraction peaks in the case of diffraction of light at a diffraction grating surface. The relation to determine the height of the potential barrier at the metal – vacuum interface was obtained.

Keywords: electrons, photons, diffraction, beam, potential barer, potential pit, discrete spectrum, elastic interaction, diffraction grating.

В роботі розглянута задача дифракції при нормальному падінні монохроматичного пучка фотонів на гратку нескінченно тонких металевих стрічок. При розв'язанні задачі використано квантово-механічний підхід до описання явища дифракції частинок. Виходячи із уявлення про пружну взаємодію фотона з електроном, що знаходиться в стрічці, і здійснює одновимірний рух в потенціальній ямі з потенціальними бар'єрами обмеженої висоти, отримано в першому наближенні співвідношення для дискретних значень кутів, під якими повинні спостерігатися дифракціїні максимуми. Показано, що рівняння, отримані в роботі, збігаються у випадку малих значень кутів дифракції світла на дифракційній гратці. Отримано співвідношення для визначення висоти потенціального бар'єра на межі метал-вакуум.

**Ключові слова**: електрон, фотони, дифракція, пучок, потенціальний бар'єр, потенціальна яма, дискретний спектр, пружна взаємодія, дифракційна гратка.

В работе рассмотрена задача дифракции при нормальном падении монохроматического пучка фотонов на решетку бесконечно тонких металлических лент. Используется квантово-механический подход к описанию явления дифракции частиц. Исходя из представления об упругом взаимодействии фотона с электроном, находящимся в ленте и осуществляющем одномерное движение в потенциалрной яме с барьерами конечной высоты, получены в первом приближении соотношения для дискретных значений углов, под которыми должны наблюдаться дифракционные максимумы. Уравнения полученные в работе, совпадают в случае малых углов дифракции с известными в научной литературе выражениями, определяющими положения дифракционных максимумов в случае дифракции света на дифракционной решетке. Получено соотношение для определения высоты потенциального барьера на границе раздела металл - вакуум.

**Ключевые слова**: Электрон, фотоны, дифракция, пучок, потенциальный баръер, потенциальная яма, дискретный спектр, упругое взаимодействие, дифракционная решетка.

#### Introduction

The article [1] offers a quantum approach to describe the diffraction of light from two slits and from periodic system of parallel slits on metal screen where they form a diffracting screen. This approach is based on the following model. Metal tape is compared to infinitely deep potential pit, slits are infinitely high barrier. Herewith, diffraction pattern composed of interleaving of minimum and maximum of illumination intensity is explained as a result of elastic interaction of photons with electrons. These electrons in strips are in the state of free movement.

This work offers a model close to reality where strips

are compared to finite depth pit and slits are compared to finite height barriers.

### Statement and solution of the problem

Supposing photon flux falls normally to the screen plane from the side of negative values X located in the YOZ plane with Y-axis slit (Fig.1). When photons pass through slits they interact with electrons of material, suppose photon deflection from rectilinear propagation is observed as a result of this interaction.

Further the following model is taken as a base. Quantum-mechanical model of grating formed by infinite



Fig. 1. Photon falling on the screen with slits.

sequence of slits (Fig.2) may be a periodic sequence of potential barriers (pits) where pits correspond to non-transparent opaque areas and barriers correspond to slits

Here we will base on the following assumptions:

1) photon passing through the slits interacts with electron;

2) electron is in the state of free movement in onedimensional potential pit with walls of finite height;

3) collision of photon with electron occurs according to the perfectly elastic collision law;

4) width of slit *b* is small compared to the width of the metal strip *a*.

It is a complicated task to produce mathematical expression of intensity distribution in the interference pattern. Here we will limit ourselves to dimension that determines the positions of the maximums.

According to the law of conservation of impulse



Fig. 2. Quantum-mechanical model of grating.

$$\vec{p}_1 + \vec{k}_1 = \vec{p}_2 + \vec{k}_2,$$
 (1)

where  $\vec{k}_1$ ,  $\vec{k}_2$  are photon impulses before and after collision,  $\vec{p}_1$ ,  $\vec{p}_2$  are impulses of electrons in metal strip before and after collision. Diagram of impulses is shown in Figure 3.



Fig. 3. Diagram of impulses of photons and electrons.

Since electron is in a plate-dimensional motion in onedimensional potential pit, it can not have X, an impulse component. Consequently, in the projections on the axis we will get

$$k_1 = k_2 \cos \vartheta, \qquad (2)$$

$$p_1 = -p_2 + k_2 \sin \theta$$

Rewrite the system of equations (2) as following

$$0 = -k_1 + k_2 \cos \theta,$$

$$p_2 = -p_1 + k_2 \sin \theta.$$

After squaring and adding we will get

$$p_{2}^{2} = k_{1}^{2} + k_{2}^{2} + 2k_{1}k_{2}\cos\vartheta + p_{1}^{2} - 2p_{1}k_{2}\sin\vartheta$$
(3)

According to the energy conservation law

$$E_{p} + E_{kl} = E_{p2} + E_{k2}, \qquad (4)$$

Where  $E_{kI}$ ,  $E_{k2}$  is total energy of photon before and after collision,  $E_{pI}$ ,  $E_{p2}$  is total energy of electron before and after collision.  $E_{p1} = \hbar \varpi_1$ ,  $E_{p2} = \hbar \varpi_2$ ,

$$E_{p1} = \sqrt{m^2 c^4 + p_1^2 c^2}$$
,  $E_{p2} = \sqrt{m^2 c^4 + p_2^2 c^2}$ , m-  
stands for mass of electron at rest

stands for mass of electron at rest.

Using binomial theorem, we get the following approximate expressions to calculate energy of photon and electron of metal strip:

$$E_{k1} = mc^{2} \left( 1 + \frac{k_{1}^{2}}{m^{2}c^{2}} \right)^{\frac{1}{2}} \approx mc^{2} \left( 1 + \frac{k_{1}^{2}}{2m^{2}c^{2}} \right)$$
$$E_{k2} \cong mc^{2} \left( 1 + \frac{k_{2}^{2}}{2m^{2}c^{2}} \right), \qquad (5)$$

$$E_{p1} \cong mc^{2} \left( 1 + \frac{p_{1}^{2}}{2m^{2}c^{2}} \right), \ E_{p2} \cong mc^{2} \left( 1 + \frac{p_{2}^{2}}{2m^{2}c^{2}} \right)$$

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Rewrite the energy conservation law (4) as following:

$$mc^{2}\left(1+\frac{k_{1}^{2}}{m^{2}c^{2}}\right)^{\frac{1}{2}}+mc^{2}\left(1+\frac{p_{1}^{2}}{2m^{2}c^{2}}\right)=$$

$$=mc^{2}\left(1+\frac{k_{2}^{2}}{2m^{2}c^{2}}\right)+mc^{2}\left(1+\frac{p_{2}^{2}}{2m^{2}c^{2}}\right)$$
(6)

After minor changes in the expression (6) we will get

$$m^{2}c^{4} + p_{2}^{2}c^{2} = m^{2}c^{4}\left(1 + \frac{k_{1}}{2m^{2}c^{2}}\right)^{2} + m^{2}c^{4}\left(1 + \frac{p_{1}^{2}}{2m^{2}c^{2}}\right)^{2} + m^{2}c^{4}\left(1 + \frac{k_{2}^{2}}{2m^{2}c^{2}}\right)^{2} + 2m^{2}c^{4}\left(1 + \frac{k_{1}^{2}}{2m^{2}c^{2}}\right)\left(1 + \frac{p_{1}^{2}}{2m^{2}c^{2}}\right) - \dots (7) - 2m^{2}c^{4}\left(1 + \frac{k_{1}^{2}}{2m^{2}c^{2}}\right)\left(1 + \frac{k_{2}^{2}}{2m^{2}c^{2}}\right) - 2m^{2}c^{4}\left(1 + \frac{p_{1}^{2}}{2m^{2}c^{2}}\right)\left(1 + \frac{k_{2}^{2}}{2m^{2}c^{2}}\right)$$

Ignoring second-order term in the expression (7) we receive

$$p_2^2 = p_1^2 + k_1^2 - k_2^2 . (8)$$

Equating right parts of (3) and (8) we will get

$$-2k_1k_2\cos\vartheta + 2p_1k_2\sin\vartheta = -2k_2^2.$$
 (9)

In the optical range the change of frequency of photon as a result of collisions with electrons (the Compton effect) is very small [3], therefore in the equation (9) can be assumed that  $k_1 \approx k_2$  and get the relation between the initial value of the impulses of interacting particles and the photon scattering angle, a diffraction angle  $\mathcal{G}$ :

$$\frac{1 - \cos \vartheta}{\sin \vartheta} = \frac{\sin \vartheta}{1 + \cos \vartheta} = \frac{p_1}{k_1}.$$
 (10)

We now determine the eigenvalues impulses of the free-electron that are moving in a symmetric potential pit with a height of potential barriers U. The spectrum of impulses / momentum of electrons, which move in the potential wells is discrete [2], and thus the deflection angles of the photons (diffraction angles) when passing through a screen with slits will also be discrete. For a given task the eigenvalues of the wave numbers can not be obtained analytically. To determine them, the transcendental equation has been obtained [2]

$$ka = n\pi - 2\arcsin\frac{k\hbar}{\sqrt{2mU}}, \quad n = 1, 2, 3, ... \quad (11)$$

where 
$$k = \frac{\sqrt{2mE}}{\hbar}$$
,  $\hbar = \frac{\hbar}{2\pi}$  is the Planck constant.

It is obvious that the movement of electrons is localized in potential pits, beyond which they can not get out, which is consistent with the idea that the free electrons in the metal are free to move in the sample, but can not go beyond it. So when we have a periodic sequence of N stripes, energy levels corresponding to a single isolated pit will not be split.

Solution of equation (11) can be obtained by iteration method. We rewrite this equation in the form

$$k\hbar = \frac{\pi n\hbar}{a} - \frac{2\hbar}{a} \arcsin\frac{k\hbar}{\sqrt{2mU}} \quad . \tag{12}$$

The first term on the right-hand side of equation (11) determines the eigenvalues of the momentum for an infinitely deep potential pit. As shown by numerical analysis, results of which are shown in Table 1, it is a good starting (zero) approximation for calculating eigenvalues of impulses (and energy levels) of the finite depth pit U. Therefore, it is better to represent it in the following form

$$p_1 = p_0 - \frac{2\hbar}{a} \arcsin \frac{p_0}{\sqrt{2mU}} , \qquad (13)$$

where 
$$p_0 = \frac{\pi n \hbar}{a}$$
,  $n = 1, 2, 3...$ 

This expression (13) shows the electron momentum in the first approximation in the pit depth U (obtained by iteration method). Equation (13) can be simplified. Assuming that in the equation  $\frac{p_0}{\sqrt{2mU_0}} \ll 1$ , we will get

$$p_{1} = p_{0} - \frac{2\hbar}{a} \frac{p_{0}}{\sqrt{2mU}} \quad . \tag{14}$$

Substituting (14) into (10) we obtain an equation of a diffraction grating

$$\frac{\sin\vartheta}{1+\cos\vartheta} = \frac{n\lambda}{2a} \left( 1 - \frac{\hbar\sqrt{2}}{a\sqrt{mU}} \right) , \qquad (15)$$

determining the position of the maxima in the diffraction pattern,  $\lambda$  is the wavelength of the incident light. For small diffraction angles  $\mathcal{G} < 1$  and a deep well (pit)  $U \rightarrow \infty$  we get the well-known equation of diffraction grating in the case of normal incidence of light [4],

$$a\sin\vartheta = n\lambda \tag{16}$$

Table 1 shows the results of numerical calculations for pit depth U = 33 eV, and width  $a = 10^{-9}$  m. It also presents the results of comparison of the values of energy  $E_{n\infty}$  and momentum  $p_{\infty}$  for the infinitely deep well with the values of energy  $E_n$  and momentum  $p_1$  for the finite depth pit that were calculated by the formula (14) in the first approximation.

In the above table also shows the values of energy  $E_n$  and momentum  $p_1$ \* for the finite depth pit, calculated by formula (12) by finding successive approximations by Newton's method. There are 9 roots in a pit at a given height of the barrier. As the table shows, the energy eigenvalues differ little from  $E_{n\infty}$  as well as  $p_{\infty}$  from  $p_1$ \* and really are a good zero-order approximation for calculating eigenvalues of momentum for the finite depth pit. Comparing the energy eigenvalues  $E_n$  with  $E_n$  (and accordingly  $p_1$ \* with p) we can see that the error does not exceed 3.5%.

According to the definition arcsin equation (12) can be written as

$$\sin\frac{p_0 - p_1}{2\hbar}a = \frac{p_0}{\sqrt{2mU}} .$$
 (17)

From equation (17) can determine the height of the potential barrier

$$U = \frac{p_0^2}{2m\sin^2\left[\frac{a}{2\hbar}(p_0 - p_1)\right]}.$$
 (18)

Suppose that we know the diffraction angles  $\, \vartheta \,$  from

the diffraction pattern obtained as the result of light diffraction on two slits or a grating formed by the N slits. In this case, the magnitude of the impulse  $p_1$  can be determined from equation (9)

$$p_1 = k_1 \frac{\sin \vartheta}{1 + \cos \vartheta} = \frac{2\pi\hbar}{\lambda} \frac{\sin \vartheta}{1 + \cos \vartheta}$$
(19)

## Conclusion

In the article the expression for calculating eigenvalues of the electron impulses in a potential well bounded by barriers of finite height has been obtained. Their estimation accuracy is given. An expression that defines the angle of diffraction, allowing finding the position of the maxima in the diffraction pattern has been obtained in the first approximation. The formula for the calculation of the potential barrier at the metal-vacuum interface has been derived.

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 $E_{n\infty}$ , eV  $E''_n$ , eV p, 10<sup>-5</sup> kGm/s  $(E''_{n} - E_{n})/E''_{n}, \%$  $E_n$ , eV  $p_{\infty}, 10^{-5} \text{kGm/s}$  $p_{1}^{*}, 10^{-5} \text{kGm} / \text{s}$  $(p-p_1)/p,\%$ n 1 0.381 0.334 0.324 3.297 3.118 3.077 1.3 2 2 1.524 1.335 1.299 6.594 6.234 6.151 1.4 2.6 5 9.528 8.301 8.123 16.49 15.55 15.32 1.5 3 9 30.87 26.32 26.32 29.67 27.66 27.11 1.9 3.5

Table 1