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Vitalii Breslavets, Igor Yakovenko, Juliya Breslavets, Vitalii Voronets

National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine

SURFACE ELECTRONIC STATES AT THE INHOMOGENEOUS INTERFACE SEMICONDUCTOR - DIELECTRIC

Abstract. The **subject matter** is the analysis processes and conditions for the generation (amplification) of electromagnetic oscillations in the submillimeter range by creating surface electronic states at an inhomogeneous interface between media, which is realized for structures such as metal – semiconductor – dielectric (M-S-D), where the localization sizes of surface states are within the range of approximately 10^{-4} cm. The **aim** is the possibility of conducting theoretical and experimental studies based on the proposed physical model for the emergence of surface electronic states at an inhomogeneous boundary of solid bodies, in conditions where the amplitude of the irregularities is much smaller than their period. Parameters of the lateral pulsed electromagnetic field, induced currents, and characteristics of semiconductor devices are established within which the mode of amplification of the intrinsic oscillations of the surface electron layer of the semiconductor structure is observed. The **objectives** are: the mechanisms of electron interaction at the interface between the conductor and dielectric, where the inhomogeneities are either random or periodic. As a result of this interaction, the electron concentration exponentially decreases with distance from the boundary. The **methods** used are: the methods of the theory of small perturbations (Rayleigh's method) to determine the spectrum of surface electronic states under conditions where the amplitude of irregularities is much smaller than their period. The following **results** are obtained: A dispersion equation for the spatial harmonics of electrons at the inhomogeneous boundary of a conducting solid body is derived. By the method of successive approximations for the small parameter, its solution is determined, and it is shown that in limiting cases—long-wavelength and short-wavelength—the localization sizes of electrons at the boundary have similar orders of magnitude for both periodic and random surfaces. **Conclusion.** The work provides quantitative estimates for the radiation energy values – the energy loss values of charged particle flows induced by an external electromagnetic field, leading to the excitation of surface electromagnetic oscillations in structures with boundary inhomogeneities in the presence of surface electronic states. The results show that the radiation energy for structures like metal – dielectric – semiconductor (M-S-D) lies in the range of $\approx (10^{-7} - 10^{-8})$ *Wt*, which is detectable by modern microwave radiation receivers (approximately 10^{-10} *Wt*).

Keywords: Rayleigh's method; inhomogeneous boundary; surface electronic states; dispersion equation; spatial harmonics; induced current; surface oscillations.

Introduction

Mastering the submillimeter and short-wavelength parts of the millimeter electromagnetic wave ranges is one of the most relevant tasks in modern radio physics. These ranges are crucial for many technical applications: communication systems, radar, radionavigation, and computing, as well as for studying the impact of external electromagnetic fields on the performance of equipment (electromagnetic compatibility (EMC) tasks). Exciting oscillations in this range requires the creation of corresponding electromagnetic radiation sources [1, 2].

Modern technology makes it possible to create conductive solid-state structures: semiconductors with two-dimensional (2D) electron gas, superlattices, as well as films and structures like metal-dielectric-semiconductor (MDS), etc. In their formation, the electronic properties of the boundary between media play a key role.

Thus, surface electronic states lead to the formation of a two-dimensional (2D) electron gas and the appearance of surface oscillations in the submillimeter range. The presence of surface electronic states at the interface between media allows the transformation of the energy of charged particle flows into energy of surface oscillations. The generation and amplification mechanisms of surface oscillations are based on Cherenkov, transition, and braking radiation effects [3, 4].

A large number of works have been devoted to the study of surface electronic states, where the main focus was on the study of electronic states arising on the surface of crystals due to the limitation of the crystal lattice or, in other words, the disruption of the periodic potential [5, 6]. Depending on the chosen physical model, Tamm states, arising from the change in the potential at the crystal-vacuum boundary, and Shockley states, caused by the break in atomic bonds at the boundary, are distinguished [7].

The two models mentioned above do not cover all problems related to surface states. Another scenario is possible when a charged particle moves in the field of a constant, rather than a periodic, potential, but its motion is limited in one direction by an inhomogeneous surface, which represents an infinitely high potential barrier.

It is known that if the boundary is homogeneous, surface states do not arise. However, for an inhomogeneous boundary, the issue of quantum surface states has not been sufficiently explored. This work investigates the possibility of surface electronic states arising due to small periodic or random inhomogeneities at the boundary of a solid body. One-dimensional roughness was used as the object of study.

The problem is solved under the condition that the scales of the inhomogeneities are small compared to the wavelengths existing in the structure. The mathematical apparatus used is based on the representation of surface roughness as small disturbances, the influence of which is taken into account in the boundary conditions.

Results

Let us consider the electronic states in a half-space $y > y_0(x)$, bounded by a potential barrier $U(x, y)$:

$$U(x,y): \begin{array}{ll} U(x,y)=\infty, & y \le y_0(x); \\ U(x,y)=0, & y > y_0(x), \end{array} \quad (1)$$

where $y_0(x)$ - is the function describing the form of the boundary between media. In this work, we limit ourselves to considering the boundary as an infinitely high potential barrier, with roughness depending on one coordinate X. The eigenfunctions $\Psi(x, y, z)$ and eigenvalues of the electron energy are determined by solving the Schrödinger equation:

$$\Delta\Psi + \frac{2m}{\hbar^2}\left[E - U(x,y)\right]\Psi = 0, \quad (2)$$

and boundary conditions at the surface and infinity. At the surface $y = y_0(x)$, boundary conditions are of two types [8]:

$$\Psi(y_0(x)) = 0 \quad (3)$$

$$\vec{n}\vec{\nabla}\Psi\big|_{y=y_0(x)} = 0; \quad \vec{\nabla} = \vec{i}\,\frac{\partial}{\partial x} + \vec{j}\,\frac{\partial}{\partial y} + \vec{k}\,\frac{\partial}{\partial z}, \quad (4)$$

where $\vec{n}$ is the normal vector to the surface $y = y_0(x)$:

$$n_x = -\frac{\frac{\partial y_0}{\partial x}}{\sqrt{\left(\frac{\partial y_0}{\partial x}\right)^2 + 1}}; \; n_y = -\frac{1}{\sqrt{\left(\frac{\partial y_0}{\partial x}\right)^2 + 1}}; \; n_z = 0, \quad (5)$$

The conditions correspond to the zero particle flux density (4) and particle density (3).

This work considers two types of boundary roughness: periodic $y_0(x) = \zeta_0\cos(Gx)$; $d = 2\pi/G$ – period of roughness) and rough $y_0(x) = \zeta(x)$, where $\zeta(x)$ is a random function. In the case of a periodically rough boundary, the wave function $\Psi(x, y, z)$ looks as follows:

$$\Psi(x,y,z) = \sum_{n=-\infty}^{\infty} A_n \exp\left[i(k_x + nG)x + ik_y y + ik_z z\right], \quad (6)$$

where $\vec{k}(k_x, k_y, k_z)$ is the wave vector of the electron.

From the Schrödinger equation (2), the relationship between E и $\vec{k}$ is as follows:

$$k_{yn}^2 = \frac{2mE}{\hbar^2} - (k_x + Gn)^2 - k_z^2 \quad (7)$$

The boundary condition (4) establishes the connection between k_x, k_{yn} and k_z, thereby defining the dispersion $E = E(\vec{k})$.

To solve the Schrödinger equation with boundary condition (4), we use perturbation theory [9], assuming that the amplitude of the roughness is small compared to its period ($\zeta_0 k_x << 1 \ll \lambda$). This allows us to limit the analysis to the harmonics $n = -1, 0, 1$, where the amplitude of the harmonic A_0 is maximum.

Substituting expression (6) into equation (4), we get the following dispersion relation:

$$k_{y0} = -\frac{1}{4}\zeta_0^2\left(\frac{\left[k_{y-1}^2 - G(k_x - G)\right]\left(k_{y0}^2 + Gk_x\right)}{k_{y-1}} + \frac{\left[k_{y1}^2 + G(k_x + q)\right]\left(k_{y0}^2 - Gk_x\right)}{k_{y1}}\right). \quad (8)$$

We will solve equation (8) using the method of successive approximations for the small parameter ζ_0: $k_{y0} = k_{y0}^{(0)} + \delta k_{y0} + \ldots$

If $\zeta_0 = 0$, then $k_{y0}^{(0)} = 0$ and

$$k_x^2 = \frac{2mE}{\hbar^2} - k_z^2. \quad (9)$$

The next approximation yields:

$$\delta k_{y0} = -\frac{1}{4}(\zeta_0 k_x G)^2\left(\frac{1}{k_{y1}} + \frac{1}{k_{y-1}}\right); \quad (10)$$

$$\delta E = \frac{\hbar^2 \delta k_{y0}^2}{2m}; \quad k_{y\pm1}^2 = -G(G \pm 2k_x). \quad (11)$$

In the case when $k_x << q$ is small, equation (10) gives:

$$\delta k_{y0} = \frac{1}{2}i(\zeta_0 k_x)^2 G; \quad k_{y1} = k_{y-1} = iG. \quad (12)$$

Solution (12) defines the localized electronic states near the surface with energy

$$E = \frac{\hbar^2}{2m}\left[k_z^2 + k_x^2\left((1 - \frac{1}{4}\zeta_0^2 G^2 k_x^2\right)\right]. \quad (13)$$

From equation (12), it is evident that the spatial localization length of the electron wave function $R = i/\left(\delta k_{y0}\right)$ decreases exponentially as the wave vector k_x increases. Thus, the electron concentration also decreases exponentially with distance from the boundary, forming a surface electron layer.

Surface inhomogeneities most effectively affect the electronic states in resonance conditions, when the wave vectors of adjacent harmonics traveling in opposite directions along the axis X coincide ($k_{y0} = k_{y-1}$). In this case, $k_x = G/2 \equiv k_r$ and from equation (10), we obtain:

$$\delta k_{y0}^2 = -\zeta_0^2 k_r^2; \quad (14)$$

$$E = \frac{\hbar^2}{2m}\left[k_z^2 + k_r^2(1 - \zeta_0^2 k_r^2)\right]. \quad (15)$$

Equation (14) has the following solutions:

$$\mathrm{Re}\,\delta k_{y0} = 0; \quad \mathrm{Im}\,\delta k_{y0} = \zeta_0 k_r^2 \qquad (16)$$

These correspond to a highly localized surface state. Thus, electronic surface states exist in the region $k_x \le G/2 - (\mathrm{Im}\,k_{y0\pm1} > 0)$.

In the region $k_x > G/2$, surface states typically do not arise. In this case, both δk_{y0} and E take on complex values. In the region $k_x >> G$ the equation (8) has the solution:

$$\delta k_{y0} = \frac{(-1+i)\zeta_0^2 (k_x G)^{3/2}}{\sqrt{2}}; \qquad (17)$$

$$\delta E = -i\frac{\hbar^2 \zeta_0^4 (k_x G)^3}{2m}. \qquad (18)$$

Thus, the quantum states are quasi-stationary, meaning they have a lifetime $\Psi \sim e^{-t/\tau}$:

$$\tau = \frac{2m}{\hbar^2 \zeta_0^4 (k_x G)^3} \qquad (19)$$

Now, let us define the mechanisms of the formation of surface electronic states when the surface roughness is random. Let the shape of the boundary surface be given by a random function $y = \zeta(x)$). Assume that $\zeta(x)$ is a stationary homogeneous process with an average value $\overline{\zeta(x)} = 0$, and its statistical properties are described by the correlation function:

$$\overline{\zeta(x)\zeta(x')} = \zeta_0^2 W(x - x') \qquad (20)$$

We assume, as in the case of periodic roughness, that the amplitude of the deviation of the random function from its mean value is small, i.e., $\frac{\partial \zeta}{\partial x} << 1 \ll \lambda$. In this case, to solve the Schrödinger equation with boundary condition (4), we can use the standard procedure to determine the field over a statistically rough surface $\zeta(x)$ [8]. After performing the necessary calculations, we obtain an expression that defines the particle spectrum:

$$k_y = -\zeta_0^2 \int_{-\infty}^{\infty} \frac{d\chi_x}{k_y}\left[k_x(\chi_x - k_x) - k_y^2\right] \times$$
$$\times\left[\chi_x(k_x - \chi_x) - \chi_y^2\right] W(k_x - \chi_x), \qquad (21)$$

where $\chi_y^2 = k_x^2 - \chi_x^2$; $k_y^2 = \frac{2mE}{\hbar^2} - k_x^2 - k_z^2$, $W(\vec{k})$ is the Fourier transform of the correlation function (20), which subsequently takes the Gaussian form:

$$W(k_x - \chi_x) = \frac{l}{2\sqrt{\pi}} \exp\left(-\gamma^2 k_x^2 L^2\right). \qquad (22)$$

Here, ℓ is the correlation $\gamma = \frac{1}{2} - \frac{\chi_x}{2} k_x$.

From equation (21), it follows that when $\zeta = 0$, we have: $k_y = 0$.

Substituting into the right-hand side of equation $k_{y0} = 0$ (21) and performing integration over the angles, we obtain δk_y, in the first approximation:

$$\delta k_y = \frac{2i\zeta_0^2 k_x l}{\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{d\gamma \gamma^{3/2} \exp(-\gamma^2 k_x^2 L^2)}{\sqrt{\gamma - 1}}. \qquad (23)$$

The solution to equation (23) can be analytically evaluated in two limiting cases: $k_x l << 1$ and $k_x l >> 1$.

In the long-wavelength limit $k_x l << 1$, the value (23) is determined by expanding the integrand in terms of the small parameter $k_x l$:

$$\delta k_y = 2i\zeta_0^2 k^2 / \sqrt{\pi} l. \qquad (24)$$

The solution to equation (24) corresponds to a localized surface state with energy:

$$E = \frac{\hbar^2}{2m}\left[k_z^2 + k_x^2(1 - 4\zeta_0^4 k_x^2 / \pi l)\right]. \qquad (25)$$

The solution to equation (23) in the long-wavelength limit implies that near the rough surface of a solid, there exist surface electronic states with a non-quadratic dispersion law. The electron wave function in this case takes the form:

$$\overline{\Psi} \sim \exp\left(-\frac{2\zeta_0^2 k_x^2}{\sqrt{\pi} l} y\right). \qquad (26)$$

In the short-wavelength limit ($k_x l >> 1$), the solution to equation (23) becomes:

$$\delta k_y = \frac{\Gamma(5/4)(1-i)}{\sqrt{\pi}} \frac{\zeta_0^2 k_x^3}{(k_x l)^{3/2}}, \qquad (27)$$

where $\Gamma(x)$ is the Gamma function. Expression (26) describes a quasi-stationary, localized electronic state near the surface with a characteristic lifetime:

$$\tau = \frac{\pi m l^3}{\Gamma^2(5/4)\hbar \zeta_0^4 k_x^3} \qquad (28)$$

Thus, small surface inhomogeneities, representing an infinitely high potential barrier, lead to the formation of surface electronic states whose function exponentially decays with distance from the boundary. The expressions that describe localized states near a rough boundary and those describing states near a periodically rough surface are analogous. In the first case, the characteristic size is the correlation length, and in the second case, it is the period of the surface inhomogeneities.

Analysis of the results obtained

The implementation of the effects mentioned can be realized, for example, at the boundary between a semiconductor and a dielectric. The boundary may have natural roughness or a periodic structure in the form of dislocation mismatches, as well as by creating an artificial periodic relief. According to the results obtained, electrons will be localized near the boundary in a layer of thickness R, since $\Psi \sim e^{-y/R}$.

In the case when the period of the surface inhomogeneity is of the order of several micrometers (microns) $a = 10^{-5}\,sm$, a value accessible by lithographic methods for structure formation, and the ratio between the amplitude of the inhomogeneity ς_0 and the wavelength $(\lambda = 1/k)$ $\varsigma_0 k \approx 0.1$, the electrons will be localized in a layer of thickness $R \approx 10^{-4}$ in the resonant case. In the long-wavelength limit, the thickness of this layer will be an order of magnitude larger.

Let us provide quantitative estimates of the conditions for the resonant (Cherenkov) interaction of surface oscillations of the surface electronic states with the flows of charged particles induced by external electromagnetic radiation, i.e., the possibilities for their generation (amplification) in current semiconductor devices used in radar and communication systems [2].

The frequency of surface plasmons for typical values of semiconductor structures used in modern radio electronics is $\omega_s \approx 10^9 - 10^{11} s^{-1}$.

The drift velocity of carriers for fields in the range E of electric and H of magnetic field strengths, affecting the semiconductor structure with surface electronic states emission, is $E < 100\frac{kV}{m};\ H < 600\frac{A}{m}$.

Therefore, the conditions for resonant interaction between waves v_f and particles (equality of the wave phase velocity and the drift velocity of the induced current $v_f = \omega_s / q \approx v_{dp}$ are satisfied for millimeter (submillimeter) wavelengths, corresponding to the size of the localization of surface electronic states $R \approx 10^{-4}$ sm.

Let us now provide quantitative estimates of the radiation energy ΔW_{rad}, i.e., the energy losses of the flow of charged particles induced by external electromagnetic fields, in exciting surface electromagnetic oscillations in structures such as metal-dielectric-semiconductor (MDS) with surface electronic states [3]. For electric fields with a field strength $E_0 \approx 10 - 50\,\frac{kv}{m}$ in the region of reversible failures, the pulse duration is $\Delta t_{imp} \approx 500\,ns$.

The concentration of carrier currents and their drift velocities lie in the range [4]:

$$n_b \approx\ 10^{10} - 10^{12}\,sm^{-3}\quad v_0 \approx\ 10^5 - 10^7\,sm/s\,.$$

The radiation energy of the own oscillations of solid-state MOS structures lies in the range $\approx (10^{-7} - 10^{-8})vm$ GHz, and thus, with the sensitivity of modern microwave radiation receivers [3] (from $10^{-10}Wt$), it is easily detectable.

Thus, the proposed physical model of the conditions for the generation (amplification) of oscillations by creating surface electronic states at an inhomogeneous interface between media is feasible for MDS structures, since the sizes of their localization are in the range of a few centimeters $R \approx 10^{-4}$ sm.

Conclusions

1. The results obtained indicate that periodic (random) inhomogeneities at the boundary between two media lead to the appearance of surface electronic states, with the concentration of electrons (wave function) exponentially decreasing with distance from the boundary.

2. It should be noted that in the limiting cases – long-wavelength and short-wavelength – the localization sizes of the electrons have the same order of magnitude for both periodic and random surfaces. The most effective interaction occurs when the de Broglie wavelength of the electron is comparable to the characteristic size of the inhomogeneity and the Bragg reflection condition is met. If the period of the surface inhomogeneities is a few micrometers, electrons will localize in a layer of thickness $R \approx 10^{-4}$ in the resonant case, and in the long-wavelength limit, in a layer an order of magnitude thicker.

3. The proposed physical model of the formation of surface electronic states at an inhomogeneous boundary can be realized in MDS structures, which creates opportunities for the generation (amplification) of oscillations in the submillimeter range, since the localization layer sizes are within a few centimeters.

Conflicts of interest

The authors declare that they have no conflicts of interest in relation to the current study, including financial, personal, authorship, or any other, that could affect the study, as well as the results reported in this paper.

Use of artificial intelligence

The authors confirm that they did not use artificial intelligence technologies when creating the current work.

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ВІДОМОСТІ ПРО АВТОРІВ / ABOUT THE AUTHORS

Бреславець Віталій Сергійович – кандидат технічних наук, доцент, професор кафедри систем інформації, Національний технічний університет "Харківський політехнічний інститут", Харків, Україна;
Vitalii Breslavets – Candidate of Technical Sciences, Associate Professor, Professor of Information Systems Department, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine;
e mail: bres123@ukr.net; ORCID Author ID: https://orcid.org/0000-0002-9954-159X;
Scopus Author ID: https://www.scopus.com/authid/detail.uri?authorId=57204843959.

Яковенко Ігор Володимирович – доктор фізико-математичних наук, професор, професор кафедри систем інформації Національний технічний університет "Харківський політехнічний інститут", Харків, Україна;
Igor Yakovenko – Doctor of Physical and Mathematical Sciences, Professor, Professor of Information Systems Department, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine;
e mail: yakovenko60iv@ukr.net; ORCID: https://orcid.org/0000-0002-0963-4347;
Scopus Author ID: https://www.scopus.com/authid/detail.uri?authorId=6601985070.

Бреславець Юлія Віталіївна – асистент кафедри систем інформації, Національний технічний університет "Харківський політехнічний інститут", Харків, Україна;
Juliya Breslavets – Assistant of Information Systems Department, National Technical University "Kharkiv Polytechnic Institute", Kharkiv, Ukraine;
e-mail: juliettar941@gmail.com; ORCID: https://orcid.org/0000-0003-4530-8028.

Воронець Віталій Миколайович – доктор філософії, доцент кафедри «Системи інформації», Національний технічний університет «Харківський політехнічний інститут», Харків, Україна;
Vitalii Voronets – PhD, Associate Professor, Department of Information Systems, National Technical University «Kharkiv Polytechnic Institute», Kharkiv, Ukraine;
e-mail: Vitalii.Voronets@khpi.edu.ua; ORCID Author ID: https://orcid.org/0000-0002-7793-3824;
Scopus Author ID: https://www.scopus.com/authid/detail.uri?authorId=58986447800.

Поверхні електронні стани на неоднородному кордоні півпровідник – діелектрик

В. С. Бреславець, Ю. В. Бреславець, І. В. Яковенко, В. М. Воронець

Анотація. Об'єктом дослідження є процес аналізу умов для генерації (посилення) електромагнітних коливань субміліметрового діапазону шляхом створення поверхневих електронних станів на неоднорідному кордоні розділу середовищ, що реалізується для структур метал – напівпровідник – діелектрик (МДП), коли розміри локалізації поверхневих станів знаходяться в межах $R \approx 10^{-4}$ см. **Мета дослідження** –можливість постановки теоретичних та експериментальних досліджень на основі запропонованої фізичної моделі виникнення поверхневих електронних станів на неоднорідному кордоні розділу твердих тіл, в умовах коли амплітуда нерівності набагато менша за її період. Встановлено параметри стороннього імпульсного електромагнітного поля, наведених струмів та характеристик напівпровідникових приладів у рамках яких спостерігається режим посилення власних коливань поверхневого електронного шару напівпровідникової структури. Методи дослідження: методи теорії малих обурень (метод Релея) при визначенні спектра поверхневих електронних станів в умовах коли амплітуда нерівності набагато менша від її періоду. **Отримані результати.** Отримано дисперсійне рівняння для просторових гармонік електронів на неоднорідній межі твердого тіла, що проводить. Методом послідовних наближень за малим параметром визначено його рішення та показано, що у граничних випадках – довгохвильовому та короткохвильовому – розміри локалізації електронів на кордоні мають однакові порядки величин як для періодичної поверхні, так і для випадкової. **Висновки.** У роботі наведено кількісні оцінки величин енергії випромінювання - величини втрат енергії потоків заряджених частинок, наведених зовнішнім електромагнітним полем, на збудження поверхневих електромагнітних коливань у структурах з неоднорідностями межі середовищ за наявності поверхневих електронних станів. Вони показують, що величина енергії випромінювання структур типу метал – діелектрик - напівпровідник лежить у діапазоні $\approx (10^{-7} - 10^{-8})$ *вт*, тобто. при чутливості сучасних приймачів НВЧ випромінювання (10^{-10} *вт*) цілком виявлена.

Ключові слова: метод Релея; неоднорідна межа; поверхневі електронні стани; дисперсійне рівняння; просторові гармоніки; наведений струм; поверхневі коливання.