A STABLE NUMERICAL ALGORITHM FOR INVESTIGATING THE PROPERTIES OF TWO-DIMENSIONAL LASER WAVEGUIDES IN MULTILAYER QUANTUM-DIMENSIONAL SEMICONDUCTOR HETEROSTRUCTURES

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Abstract. The transfer of heat through nanostructures differs significantly from the corresponding processes inside macroscopic bodies. Various research methods, both theoretical and experimental, are applied to such objects. This approach to nanostructures gives great advantages. The hyperbolic equations we have obtained describe the wave process of the thermal signal flow and the properties of heat transfer in nanostructures across a thin layer, in which the simplest task is to determine the thermal conductivity.

1. Introduction
Multilayer nanostructures are artificially formed layered structures consisting of a large number (up to tens of thousands) of alternating nanolayers of various materials. The list of materials used to create multilayer nanostructures is quite wide – it can be pure metals, alloys, semiconductor materials, materials with dielectric properties in various combinations. The thickness of the layers of multilayer nanostructures, as a rule, is in the range from 1 to 100 nm. It is worth noting that the greatest interest is the study of multilayer nanostructures with layers of thickness from units to several tens of nanometers. This is due to the fact that it is in this range that the degree of influence of the dimensional factors of nanolayers on the structure and properties of materials acquires the greatest importance. Thus, the ultra-small thickness of the layers in combination with a large number of interfaces between the layers and the alternation of layers of different materials leads to the appearance of multilayer nanostructures with unique structural features that are not present in the materials that make up the nanostructures in massive samples [1]. The manifestation of such features is associated with the detection of such physical properties in multilayer nanostructures as extremely high hardness [2], low transverse thermal conductivity [3], the effect of giant magnetoresistance (GMR) [4], divergence of the radiative characteristics of heterolasers with increasing temperature [5-8], etc.

Heteronanolasers have high radiative characteristics and different variants, for example, strained quantum-dimensional heterostructures, which are currently being actively investigated [5-10].

Today's technologies for the production of semiconductor lasers make it possible to grow quantum-sized heterostructures with dozens of layers, which, in any case, requires a more natural description of
the parameters of their structures in terms of the temperature dependence of the radiative characteristics. Previously developed models do not always provide the required accuracy.

In [11-13], on the example of multilayer planar optical waveguides, the waveguide properties of which are determined not by the total internal reflection from the core-shell boundary, as in conventional optical waveguides, but by the antiresonance reflection from the multilayer shell, ARROW waveguides, the effectiveness of a new numerical method for calculating the spectrum and attenuation coefficient of the resulting electromagnetic modes is demonstrated. The method proposed in [11-13] is equally applicable both to the calculation of electromagnetic modes in dielectric waveguides and to the calculation of quantum states of electrons in multi-barrier semiconductor heterostructures. The results of comparing the characteristics of multilayer waveguides calculated on the basis of the proposed method with the known ones obtained by solving a complex dispersion equation within the framework of the transfer matrix method are presented. As an example, the results of calculating the spectral dependence of the radiation attenuation of the first flowing TE mode of a planar optical waveguide with 52 pairs of layers are given.

The authors of [5, 6] for the first time experimentally detected a decrease in the divergence of InGaAs-heterolaser radiation with an increase in temperature. Based on the model of a waveguide with varying parameters, a calculation is made that allows us to explain the temperature decrease in the width of the radiation pattern and the increase in the threshold current. The results of the work are determined in favor of a waveguide mechanism for abnormal temperature growth of the threshold current of long-wave InGaAs-heterolasers.

The paper [13] presents a simple matrix technique for calculating the radiation characteristics of various modes, including losses for an arbitrary stepped planar waveguide structure with complex refractive indices.

In this regard, this article proposes a new approach to the development of a more convenient and optimal method for numerical calculation of the properties of the waveguide of heterostructures, which allows optimizing the temperature dependence of the intensity distribution in the far field of injection lasers at different parameters of nanostructures.

2. A model study of the characteristics of two-dimensional laser waveguides

It is known [10] that the electromagnetic field in the medium is determined by Maxwell’s equations:

\[ \nabla \times E = -\mu \frac{\partial H}{\partial t}, \quad \nabla \cdot H = 0, \]  
\[ \nabla \times H = \varepsilon \frac{\partial E}{\partial t}, \quad \nabla \cdot E = 0, \]  

where \( E, H \) are the electric and magnetic field strengths, respectively; \( \mu \) is the magnetic permeability, and \( \varepsilon \) is the dielectric constant of the medium.

As is known [10] (see page 155), the electromagnetic field propagating in a vacuum is called an electromagnetic wave. Vector \( E \) and \( H \) satisfy the wave equation:

\[ \Delta E - \mu \varepsilon \frac{\partial^2 E}{\partial t^2} = 0, \]  
\[ \Delta H - \mu \varepsilon \frac{\partial^2 H}{\partial t^2} = 0, \]  

where \( v = \frac{1}{\sqrt{\varepsilon \mu}} \) is the velocity of propagation of an electromagnetic wave in a material medium. The propagation velocity of an electromagnetic wave in a medium is related to the propagation region in a
vacuum by the expression: 
\[ \varepsilon' = \frac{c}{\varepsilon} \]
In this expression, \( \varepsilon' \) is the relative permittivity. The relative permittivity is related to the refractive index by the expression: 
\[ n = \sqrt{\varepsilon'} \]

The task is to study the influence of the field propagating along the axis on the nature of the change in the components \( E_x \) and \( E_y \) of the field. Suppose that an electromagnetic wave in a semiconductor laser propagates along the axis \( Oz \). Then, for example, equation (3) for the electric field strength can be divided into two equations:
\[
\frac{\partial^2 E_x(x, y, t)}{dx^2} - \mu \varepsilon \frac{\partial^2 E_x(x, y, t)}{dt^2} = 0, \\
\frac{\partial^2 E_y(x, y, t)}{dy^2} - \mu \varepsilon \frac{\partial^2 E_y(x, y, t)}{dt^2} = 0.
\]

We will look for the general solution of equations (4) and (5) in the following form:
\[
E_x(x, y, t) = E_x(x, y) \exp( i( \omega t + \beta z ) ), \\
E_y(x, y, t) = E_y(x, y) \exp( i( \omega t + \beta z ) ),
\]
where \( \omega \) is the frequency of the electromagnetic field oscillation.

In multilayer semiconductor laser structures, only the polarization \( TE \) modes are considered. This is due to the fact that TM modes have significantly greater attenuation than \( TE \) modes. In the \( TE \) modes of polarization the only spatial component \( E_z(x, y) \) is different from zero.

Thus, according to (4), (5) and (6), the wave function can be searched for as a multiplication of two functions:
\[
E_z(x, y, t) = E_z(x, y) E_z(y),
\]
each of which satisfies the one-dimensional Helmholtz equation:
\[
\frac{d^2 E_z(x)}{dx^2} + q_1^2 E_z(x) = 0, \quad q_1 = \sqrt{\beta_x^2 - \frac{1}{2} n_0^2 k_0^2}, \\
\frac{d^2 E_z(y)}{dy^2} + q_2^2 E_z(y) = 0, \quad q_2 = \sqrt{\beta_y^2 - \frac{1}{2} n_0^2 k_0^2},
\]
where \( (x, y) \) is the coordinate along the transverse axis to the layers, \( k_0 = \frac{\omega}{c} \) is the wavenumber in vacuum, \( \omega \) is the frequency of optical radiation, \( \varepsilon = n^2 \) is the complex permittivity, \( n \) is the complex refractive index, \( \beta_x = \beta_x + \beta_y \) is the longitudinal propagation constant, \( E_z(x) \), \( E_z(y) \) are the amplitude profiles of modes – own functions (OF). It is enough to solve one of these equations to write a solution for the others by analogy.

The solution of equation (7) ((8)) makes it possible to determine a singular point in the phase plane. Depending on the value of \( \beta_x, \beta_y \) - the complex wave propagation constant, it is possible to have an infinite number of equilibrium states, that is, for equation (7) ((8)) there are an infinite number of solutions that can be in the far field of multilayer injection lasers or near.

The constant factor at 
\[ q_1 = \sqrt{\beta_x^2 - \frac{1}{2} n_0^2 k_0^2} \]
is equal to one here, which is possible if we choose the scale along the x axis accordingly. Let the potential be a given piecewise continuous real periodic function with a period \( T \):
\[
E_z(x + T) = E_z(x).
\]
We are looking for the eigenvalue of $\beta_l$, the longitudinal constant of wave propagation, for which the differential equation has an identically non-zero solution of $E_z(x)$ and which remains bounded for all real $x$.

We use matrix calculus for the sake of clarity. Let $E_1^z(x)$, $E_2^z(x)$ be a system of fundamental functions of equation (7). Then, due to the periodicity of the differential equation $E_1^z(x+T)$, $E_2^z(x+T)$ are also solutions: they can therefore be represented as linear combinations of $E_1^z(x)$, $E_2^z(x)$:

$$
\begin{align*}
E_1^z(x+T) &= C_{11}E_1^z(x) + C_{12}E_2^z(x), \\
E_2^z(x+T) &= C_{21}E_1^z(x) + C_{22}E_2^z(x).
\end{align*}
$$

The Wronskian of this system has a value independent of $x$ and nonzero:

$$
\begin{vmatrix}
E_1^z(x+T) & E_2^z(x+T) \\
E_1'(x+T) & E_2'(x+T)
\end{vmatrix} = \begin{vmatrix}
E_1^z(x) & E_2^z(x) \\
E_1'(x) & E_2'(x)
\end{vmatrix} \cdot \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix}.
$$

Therefore,

$$
C_{11}C_{22} - C_{12}C_{21} = 1. \tag{10}
$$

If you enter a column vector

$$
\delta_k = \begin{bmatrix} E_1^z(x + kT) \\ E_2^z(x + kT) \end{bmatrix}
$$

and a matrix of coefficients

$$
D = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix},
$$

then (8) can be written as:

$$
\delta_k = D \cdot \delta_{k-1} = D^2 \cdot \delta_{k-2} = \ldots = D^k \cdot \delta_0. \tag{11}
$$

Here $D$ is a degenerate matrix, (11) valid for all integer (also negative) values of $k$.

Let $\eta_1, \eta_2$ be the characteristic numbers of the matrix $D$, that is, by virtue of (10) the root of the equation:

$$
q^2 - q(\eta_1 + \eta_2) + 1 = 0. \tag{12}
$$

Then we can deduce from the matrix calculus theorem:

a) If $|\eta_1 + \eta_2| > 2$, then the roots $q_1, q_2$ are real, their multiplication is 1, that is, in particular, if $|q_1| > 1$, then $q_2 < 1, D^k \cdot \delta_0$ for $k \to \infty$ or $k \to -\infty$ is unlimited; the corresponding value $\beta_l$ is not an eigenvalue in this case.

b) If $|\eta_1 + \eta_2| < 2$, then the roots $q_1, q_2$ are complex conjugate, $|q_1| = |q_2| = 1, D^k \cdot \delta_0$ for any $\delta_0$ remains bounded; each solution of equation (7) is an eigenfunction; the corresponding quantities $\beta_l$ are doubly degenerate eigenvalues.

c) If $|\eta_1 + \eta_2| = 2$, that is $\eta_1 + \eta_2 = \pm 2$, there is at least one vector $\delta_0$ satisfying equality $D \cdot \delta_0 = \pm \delta_0$, that is, a solution $E_z(x)$ of equation (7) having the property $E_z(x + T) = \pm E_z(x)$.

Then there is equality $E_z(x + 2T) = E_z(x)$.

The general solution of the first equation in the inner domain has the form:
\[ E_z(x) = C_1 \exp(q_1 x) + C_2 \exp(-q_1 x). \]  

(13)

The first term in (13) describes the free movement of the wave in the positive direction of the \( x \) axis, and the second in the opposite direction. The squares of the modules of the coefficients \( C_1 \) and \( C_2 \) are equal to the probabilities of detecting a wave in the corresponding states.

According to the problem statement, the wave function should vanish at the boundary of these regions. The derivative of the wave function at such a boundary may experience a jump. When solving equation (7), the boundary conditions at infinity must be correctly set. In this case, all wave propagation processes can be divided into two classes:

1) the negligible probability of the wave staying at infinity, in which the wave function can be normalized by one condition:

\[ \int |E(r)|^2 \, dV = 1. \]  

(14)

2) the wave state is finite, the probability of staying in infinity is nonzero. In this case, one can see by example the propagation of a wave in a limited volume (quantum well) of the simplest geometric shape (see Fig. 1 in [11]):

\[ 0 \leq x \leq d, \quad 0 \leq y \leq b. \]

The specified conditions for the propagation of an electromagnetic wave will be met at the following potential:

\[ E_z(x, x) = \begin{cases} 0 & \text{inside the rectangle,} \\
\infty & \text{outside the rectangle.} \end{cases} \]

Boundary conditions 2) on the walls of the parallelepiped \( E_z(0) = 0, \quad E_z(d) = 0 \) lead to the following relations:

\[ \begin{cases} C_1 + C_2 = 0, \\
C_1 \exp(q_1 d) + C_2 \exp(-q_1 d) = 0. \end{cases} \]

According to the third condition c) of matrix calculus, the wave eigenfunction has the form:

\[ E_z(x) = C_1 (\cos(q_1 x) - \sin(q_1 x)) + 2 \sin(q_1 x). \]

According to the second one, it is possible to find the eigenvalue of the wave vector and the energy of one-dimensional motion:

\[ q_{1,1} = \frac{2}{3 + \sqrt{2}}, \quad q_{1,2} = \frac{2}{3 - \sqrt{2}}, \quad \beta_x = \sqrt{q_{1,1}^2 - \frac{1}{2} n^2 k_0^2}, \]

where \( n \) is any integer greater than or equal to zero.

Conditions (2) can be satisfied if we normalize each one-dimensional function by one. From here we have:

\[ 1 = \int_0^d |E_z(x)|^2 \, dx = C_1^2 \left( a + \frac{1}{q_1} \sin^2(q_1 a) \right) + 2 C_1 \left( \frac{1}{q_1} \sin(q_1 a) \left( \cos(q_1 a) - \sin(q_1 a) \right) + a - \frac{2}{q_1} \sin(q_1 a) \cos(q_1 a) \right). \]

It follows that:

\[ C_1^2 (q_1 a + \sin^2(q_1 a)) + 2 C_1 \left( \sin(q_1 a) \left( \cos(q_1 a) - \sin(q_1 a) \right) - q_1 a \right) + 2 (aq_1 - \sin(q_1 a) \cos(q_1 a)) - q_1 = 0. \]

where
In the second region of stabilizing the temperature dependence of the radiation, we have:

\[
\frac{d^2 E_{z3}}{dx^2} + q_{x3}^2 E_{z3}(x) = 0, \quad q_{x3} = \sqrt{\beta_{x3}^2 - \frac{1}{2} n^2 k_0^2},
\]

\[
E_{z3}(x) = C_3 \exp(i q_{x3} x) + C_4 \exp(-i q_{x3} x).
\]

To satisfy the normalization condition, the condition of the wave function decreasing at \(x \to \infty\) is necessary so that \(C_4 = 0\).

The boundary value at \(x=0\) gives the ratio:

\[
C_1 + C_2 = 0. \tag{15}
\]

For \(x=a\), the wave function and its derivative must be continuous, that is, they must be crosslinked:

\[
E_{z2}(a) = E_{z3}(a), \quad \frac{dE_{z2}(x)}{dx} \bigg|_{x=a} = \frac{dE_{z3}(x)}{dx} \bigg|_{x=a}. \tag{16}
\]

The conditions of "crosslinking" (15), considering (14), give the following relations:

\[
2i C_1 \sin(q_{x2} a) = C_3 \exp(q_{x3} a), \quad 2i C_1 q_{x2} \cos(q_{x2} a) = C_3 q_{x3} \exp(q_{x3} a). \tag{17}
\]

From these relations and the normalization conditions, the coefficients \(C_1, C_3\) and the modulus of the wave vector \(q_{x2}\) can be found. By dividing the ratios (17) one by the other, it is possible to exclude the coefficients \(C_1, C_3\) and determine the following transcendental equation for \(q_{x2}\):

\[
tg(q_{x2} a) = \frac{q_{x2}}{q_{x3}}.
\]

Thus, for the value of the propagation constant and the wave function of a two-dimensional waveguide, we have:

\[
\beta_x = \beta_{x1} + \beta_{x2} = \sqrt{q_{x1}^2 - \frac{1}{2} n^2 k_0^2} + \sqrt{q_{x2}^2 - \frac{1}{2} n^2 k_0^2},
\]

\[
E_z(x,y) = E_z(x)E_z(y),
\]

where \(n=0,1,2, \ldots\).

The algorithm for calculating the task with the help of computer modeling allows optimizing the parameters of multilayer semiconductor injection lasers based on heterostructures from the point of view of stabilizing the temperature dependence of the radiative characteristics of these types of lasers. Calculation of the intensity distribution of laser radiation in the near and far field, considering the
temperature regime, allows to increase the efficiency of radiation input into optical cables of special laser models.

3. Conclusion

The new approach allows us to consider the influence of the temperature mode of operation of semiconductor quantum-dimensional injection lasers on their radiative characteristics and quantum semiconductor nanostructures. It is based on two ideas: the replacement of the traditionally used Transfer Matrix Method (TMM) with the exact analytical method proposed by us and the use of a new method for calculating the attenuation coefficient of the resulting modes, approximate, but asymptotically tending to be accurate with decreasing attenuation.

The possibility of accurate calculation of multilayer ARROW waveguides is extremely important, in particular, for their prospective application as elements of optical integrated devices. Other paragraphs are indented (BodytextIndented style).

Low-temperature plasma can be used for the synthesis of various nanostructures and is well suited for the modification of various surfaces. This is shown in many works [16-35].

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