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Dispersion of a double metal waveguide of a quantum cascade laser in the optical phonon region of GaAs

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> Analytical calculations of the dispersion characteristics of the guided modes in a double metal (DM) waveguide of a quantum cascade laser (QCL) in the optical phonon region in GaAs based on the modified Marcatili method are presented. The calculation results correlate well with the results of the numerical solution of the Helmholtz equation at optical phonon frequencies of GaAs. It is shown that the dominant mode E_{00}^{y} far from the phonon resonance of GaAs ceases to be such for frequencies near this resonance, what makes E_{10}^{y} mode the dominant mode at these frequencies.

> Keywords: terahertz frequency, terahertz lasers, semiconductors, quantum cascade laser, dispersion, waveguide, Marcatili method.

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Quantum cascade lasers (QCLs) with a double metal (DM) waveguide have the capability to generate radiation in the range from 2 to 5 THz with a peak power at the level of several tens of mW [1,2]. As was demonstrated recently in [3], the use of a DM waveguide allows one to raise significantly the QCL operating temperature (up to 261 K).

In the present study, we propose a theoretical approach based on a modification of the Marcatili method for analytical calculation of the mode composition and dispersion of a QCL DM waveguide in the optical phonon frequency region of GaAs. The dispersion of a laser waveguide is an important parameter that is needed to determine a number of quantities, such as group velocity of light v_{gr} . Since v_{gr} is inversely proportional to the probability of stimulated emission, it becomes possible to increase the laser gain by reducing v_{gr} (e.g., via the photonic crystal environment of a waveguide [4]). The proposed approach incorporates the OCL permittivity calculation in the effective medium approximation, which allows for a more accurate determination of the effective permittivity with account for the contribution of both AlGaAs barriers and GaAs quantum wells. In addition, a QCL is a uniaxial medium in the indicated approximation. This has a significant effect on the dispersion (especially near phonon resonances) and is also taken into account in the proposed model. Numerical modeling of the two-dimensional Helmholtz equation was performed for comparative analysis using the finite element method (FEM) with similar material parameters.

The schematic diagram of a QCL with a DM waveguide is shown in Fig. 1. The original Marcatili method [5] was adapted to a DM waveguide with consideration of the boundary conditions in which the metal layer in the waveguide is an ideal conductor (the tangential electric field component is zero, $E_t = 0$). Another change is related to the nonuniformity of the dielectric tensor included in Maxwell's equations in the effective medium approximation ($\varepsilon_{xx} = \varepsilon_{zz} = \varepsilon_{\parallel}$ and $\varepsilon_{yy} = \varepsilon_{\perp}$). Having performed mathematical transformations similar to the ones from the original paper [5] (but differing in that all the mentioned modifications were added), we obtained the following transcendental equation for



Figure 1. Schematic diagram of a QCL with a DM waveguide. Metal contacts adjacent to the active region (blue) are shown in gold. The cross section of a waveguide with width w and height d is located in plane (xy), and the guided mode propagates along the z axis. A color version of the figure is provided in the online version of the paper.



Figure 2. Dispersion of modes E_{00}^{y} and E_{10}^{y} in a QCL DM waveguide (*a*) and distribution of component $|E_{y}|$ of the electric field of modes E_{00}^{y} and E_{10}^{y} (*b*) near the phonon resonance in GaAs. The waveguide considered in solving the Helmholtz equation by FEM has an active region with width $w = 100 \,\mu\text{m}$ and height $d = 10 \,\mu\text{m}$.

modes E_{mn}^{y} :

$$k_{x}w = \pi n$$

- 2 arctan $\left(\frac{k_{\parallel}^{2}(k_{0}^{2} - k_{y}^{2})}{k_{0}^{2}(k_{\parallel}^{2} - k_{y}^{2})} \times \frac{k_{x}}{\sqrt{k_{\perp}^{2} - k_{0}^{2} - k_{x}^{2} - (\frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}} - 1)k_{y}^{2}}}\right),$
(1)

where component $k_y = \frac{\pi m}{d}$, w is the waveguide width, d is the waveguide height, k_0 is the wavenumber in vacuum, and $k_{\perp,\parallel}^2 = \varepsilon_{\perp,\parallel} k_0^2$, n and m — nonnegative integers; axis y is perpendicular to the contacts and QCL layers, while axes xand z are parallel to them. In this case, $\varepsilon_{\perp,\parallel}$ — permittivity of the GaAs/AlGaAs active region in the effective medium approximation for a flat layered structure, where the ε value for each layer is calculated within the Drude–Lorentz [6] model with GaAs [7] material parameters for quantum wells, while the Al_{0.15}Ga_{0.85}As parameters for barriers are derived from the Clausius–Mosotti relation or linear interpolation (Vegard's law) through the GaAs and AlAs [8,9] material parameters. The phonon resonance width for both materials was taken to be equal to 0.1 meV [10]. The electron density in cascade layers is $n = 10^{16} \text{ cm}^{-3}$. If components k_x and k_y are known, it is easy to determine propagation constant $\beta = \sqrt{k_{\perp}^2 - k_x^2 - \frac{\varepsilon_{\perp}}{\varepsilon_{\parallel}}k_y^2}$, the frequency dependence of which $(\beta(\omega))$ is the inverse dispersion. All parameters were calculated for the cascade design from [11] with widths of 41/**136**/43/75.6/24.6/**69.3** Å, where the widths of GaAs quantum wells are given in bold type and the widths of Al_{0.15}Ga_{0.85}As barriers are given in light type.

The dispersion of a DM waveguide with typical terahertz QCL width $w = 100 \,\mu\text{m}$ and height $d = 10 \,\mu\text{m}$ values for modes E_{00}^{y} and E_{10}^{y} is presented in Fig. 2, *a* at frequencies close to the phonon resonance in GaAs. At a frequency of ~ 8.15 THz, the E_{10}^{y} mode dispersion crosses the curve for E_{00}^{y} , and mode E_{10}^{y} then remains dominant through to 8.22 THz. This change of the dominant mode is associated with the high permittivity of the active QCL region and is attributable to the fact that component $k_y = \frac{\pi}{d}$, which dominates over all other parameters of the dispersion equation at lower frequencies, is no longer prevalent at frequencies corresponding to the phonon resonance in GaAs. This is the reason why the E_{10}^{y} mode in the lowfrequency region is considered to be a mode of such a high order that its excitation in a waveguide is virtually impossible; consequently, it was not considered in earlier calculations of DM waveguide modes. The distribution of the electromagnetic field of modes E_{00}^y and E_{10}^y in the cross section of the DM waveguide calculated using the modified Marcatili method and FEM is presented in Fig. 2, b for the E_v field component. It can be seen that the spatial distribution of the field calculated analytically agrees accurately with the numerical solution.

Thus, a modified analytical method for calculating the modes of a QCL with a DM waveguide in the Marcatili approximation was demonstrated. This method allows one to calculate quickly (and within a wide frequency range) the dispersion and distribution of the electromagnetic field inside a DM waveguide. The results of calculation may be used as input data for solving the Helmholtz equation by FEM to find the modes of a given order. It was found that the E_{10}^{y} mode exists near the phonon resonance. This mode remains dominant within a certain neighborhood of it.

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Conflict of interest

The authors declare that they have no conflict of interest.

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