

# Antiresonant Reflecting Optical Waveguide-Type Vertical-Cavity Surface Emitting Lasers: Comparison of Full-Vector Finite-Difference Time-Domain and 3-D Bidirectional Beam Propagation Methods

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**Abstract**—The cold-cavity modal characteristics of an antiresonant optical waveguide-type cylindrical vertical-cavity surface-emitting laser (VCSEL) are investigated through numerical simulations using a three-dimensional (3-D) bidirectional beam propagation method (BD-BPM) and a full-vector axisymmetric finite-difference time-domain (FDTD) method. Good agreement between the BPM- and FDTD-computed radial mode profiles as well as the mode-dependent radiation losses is obtained. The results of this paper establish the accuracy of the BD-BPM technique for simulating this class of devices and confirm effective-index method predictions that antiresonance conditions for cylindrical geometry devices (i.e., VCSELs) differ from those of planar geometry devices (i.e., edge emitters).

**Index Terms**—Beam propagation method, finite-difference time-domain (FDTD) method, vertical-cavity surface-emitting laser (VCSEL).

## I. INTRODUCTION

VERTICAL-CAVITY surface-emitting lasers (VCSELs) possess a low-gain (the active layer thickness is tens of nanometers) and highly reflective Bragg mirrors consisting of alternating layers of quarter-wave-thick high- and low-refractive index epitaxial materials. These lasers draw much attention due to ease of manufacturing, rather low-lasing threshold, and comparatively low-beam divergence. The ability to achieve high-power single-mode VCSELs is of great interest for many applications such as telecommunications, optical

storage, and laser printing, etc. The conventional small-aperture (diameter  $< 4 \mu\text{m}$ ) VCSELs are limited in a single-mode power to about 5 mW [1]. Attempts to increase continuous wave (CW) output powers met the problem that a larger waveguide generally supports multiple modes. Recently, several approaches [2]–[5] exhibited about 6-mW single-mode output from large-aperture ( $> 8 \mu\text{m}$ ) positive-index guided (oxide-confined) VCSELs. Another option to achieve a large spot-size single-mode operation is the usage of negative-index waveguides (antiguides) with a large built-in modal discrimination (higher order modes have significantly higher edge radiation losses). Although antiguided VCSELs have been demonstrated to be capable of operating single mode up to very high-driving currents [6]–[9], output powers were low, due to the high-edge radiation losses for the fundamental mode.

In order to reduce the edge radiation losses the reflectors can be introduced, which at the antiresonant conditions, similar to the VCSEL's longitudinal distributed Bragg reflectors (DBRs) case, minimize lateral radiation. These types of structures are generally called antiresonant reflecting optical waveguide (ARROW) [10] and have been recently proposed and demonstrated [11]–[13]. To optimize the design of this promising device, numerical modeling is of great value.

An effective index model [14] and fiber mode approximation (EI-FMA) were implemented to design a simplified ARROW (S-ARROW) [11] and an ARROW-type VCSEL [13]. In these models, the cylinder configuration was approximated by a planar geometry. Tee *et al.* [15] improved upon this approach by introducing the cylindrical geometry into the EI-FMA framework. They solved a two-dimensional (2-D) wave equation with the radial EI profile found by the approximate separation of vertical and in-plane variables [14]. It was shown in [15] that accounting for the cylindrical geometry leads to a down shift of the antiresonant width of the antiguided ring. An ARROW VCSEL with two cylindrical Bragg-like pairs (double ARROW) was also analyzed using the EI-FMA technique [16]. It was shown that for the double-ARROW device, the best discrimination of the fundamental mode against higher order modes is achieved when widths of low-index layers are chosen

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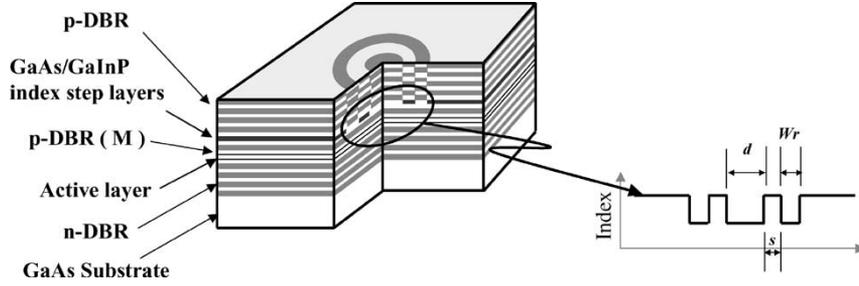


Fig. 1. Schematic diagram showing the interior cross section of an ARROW VCSEL structure.

properly. All these studies were restricted to considerations of the cold-cavity optical modes.

A recent EI-FMA analysis of an active cylindrical ARROW VCSEL [17] showed the importance of spatial hole burning (SHB) and thermal lens effects in the suppression of higher order modes. However, it is not evident that the EI-FMA is sufficiently rigorous for analyzing such effects. An alternative and more accurate approach based on the three-dimensional (3-D) bidirectional beam propagation method (BD-BPM) [18], [19] was applied to above-threshold modeling of large aperture 2-D antiguided VCSEL arrays [20]. While the BD-BPM is 10–100 times slower than the EI-FMA, it offers the potential for a greater accuracy since it is free of additional approximations required to apply the EI-FMA for above-threshold simulations. It is of interest to establish the accuracy of 3-D BD-BPM relative to more rigorous but also more computationally costly full-wave computational electromagnetics techniques.

In this paper, we investigate the accuracy of the 3-D BD-BPM in computing the cold-cavity modal characteristics of an ARROW-type cylindrical VCSEL. A full-vector axisymmetric finite-difference time-domain (FDTD) technique [12], [21] is used as the benchmark in this paper. From this paper, we can draw conclusions about the accuracy of the BD-BPM and gain confidence in the results generated from BD-BPM numerical simulations of structurally complex passive and active VCSEL devices.

## II. ARROW VCSEL DESIGN

As shown in Fig. 1, the ARROW VCSEL is composed of transversely uniform layers forming *p*- and *n*-DBRs and thin ring-shaped spacer layers located at some distance from the cavity, which includes three quantum wells (QWs) surrounded by spacers and cladding layers. Parameters of the simulated structure are listed in Table I. The important structural design parameters studied in the paper are 1) the number of DBR pairs *M* separating the  $\lambda$ -cavity and the spacer layers that form the built-in index step; 2) the low-index core diameter *d*; and 3) the high-index reflector width *s*.

## III. FDTD METHOD

Full-vector FDTD solutions of Maxwell's equations in cylindrical coordinates [21] are useful for investigating a transverse mode selectivity in complex VCSEL structures, as demonstrated previously for air-post index-guided and S-ARROW

VCSELS [12], [22]. The FDTD method permits a highly accurate analysis of the resonant frequencies, quality factors (*Q*), which are inversely proportional to the mode-dependent lateral-radiation losses, and the transverse modal profile at any resonant frequency. Since the ARROW VCSEL exhibits rotational symmetry, the azimuthal ( $\phi$ ) dependence of the vector field components can be expressed as a Fourier series and accounted for analytically, eliminating the need for gridding in the  $\phi$ -direction. The FDTD simulation is simply rerun for each azimuthal mode of interest. In this paper, we focus on modes with an azimuthal mode number of  $m = 1$ , since those modes are expected to exhibit the smallest radiation losses. In this case, the field variation along the azimuthal direction can be described simply by  $\{E_\rho(\rho, z), E_z(\rho, z), H_\phi(\rho, z)\} \cos(\phi)$  and  $\{H_\rho(\rho, z), H_z(\rho, z), E_\phi(\rho, z)\} \sin(\phi)$ . The intensity pattern for this mode is independent of  $\phi$ . The resonant frequency and *Q*-factor of each transverse mode were obtained via spectral analysis of the time-domain impulse response of the cold-cavity VCSEL structure. To significantly reduce the simulation time required to accurately extract resonant frequencies and *s*, we processed the early-time response using a Padé/fast Fourier transform (FFT) linear extrapolation scheme [21]. The modal identity of the cavity resonance was obtained from a knowledge of the azimuthal mode number assumed in the simulation and from observations of the transverse modal profile for a single-frequency source excitation at the resonant frequency.

## IV. THREE-DIMENSIONAL BD-BPM

The 3-D BD-BPM developed in [18] and [19] was applied to model the ARROW-type VCSEL structure. The 3-D BD-BPM calculations provide estimates of the modal frequencies and losses, as well as modal patterns in the near- and far-fields. The scalar wave equation for optical field amplitude *U*

$$\Delta U + k_0^2 (n(x, y, z))^2 U = 0 \quad (1)$$

was solved numerically. Here,  $k_0$  is the reference wavenumber;  $n(x, y, z)$  is the refractive index. A short description of the method is as follows. The wave field within blocks of the uniform layers was decomposed into an angular spectrum of plane counter-propagating waves with help of the FFT technique. Then, a well-known transfer matrix method for each Fourier component of the wave field within the plane layered structure

TABLE I  
STRUCTURAL SPECIFICATIONS FOR SIMULATED VCSEL

part of the construction		material	n	thickness, $\mu\text{m}$
Cap layer		GaAs	3,512	0,07
P-DBR	20.5pairs	$\text{Al}_{0,15}\text{GaAs}$	3,442	0,072
		AlAs	3,007	0,081
Regrowth $h(\lambda/2)$		GaAs	3,512	0,14
Index step		GaAs	3,512	0,006
		InGaP	3,17	0,008
p-DBR	2/3 pairs	GaAs	3,512	0,07
		AlAs	3,007	0,081
Cavity		$\text{Al}_{0,25}\text{GaAs}$	3,366	0,113
		GaAs	3,512	0,01
		$\text{In}_{0,18}\text{GaAs}$	3,6	0,007
		GaAs	3,512	0,01
		$\text{In}_{0,18}\text{GaAs}$	3,6	0,007
		GaAs	3,512	0,01
		$\text{In}_{0,18}\text{GaAs}$	3,6	0,007
		$\text{Al}_{0,25}\text{GaAs}$	3,366	0,113
n-DBR	30 pairs	AlAs	3,007	0,081
		GaAs	3,512	0,07
Substrate		GaAs	3,512	

[18] was applied to calculate the wave field after upward and downward round-trips starting from the spacer layer. In this way, the distributed reflection was described adequately. The thin spacer layer was treated as a screen with a transversely modulated phase advance  $\varphi(x, y)$ . We described transmission of the wave field through this screen by performing the inverse Fourier transform and multiplying the amplitude by an exponential factor dependent on the designed phase advance:  $\exp[i\varphi(x, y)]$ . Such a methodology allows us to calculate optical modes with a high rate not unattainable in other methods.

The FFT technique was used for the evaluation the 2-D Fourier transform and its inversion  $\mathbf{F}^{-1}$ . The spectrum of spatial frequencies of the plane waves incorporated into calculations was cut by some maximum value, which was evaluated from a compromise between the convergence problem and the accuracy of simulations.

To compute optical modes and their losses, a round-trip operator  $\mathbf{P}$  was built up, which includes propagation of the

wave field over the cavity,  $p$ - and  $n$ -Bragg mirrors, and transmission through the spacer layer with a variable thickness. The procedure of constructing the round-trip operator is described in detail in [18], [19]. Thus, we have to solve the eigenproblem for the  $\mathbf{P}$  operator

$$\mathbf{P}u = \gamma u. \quad (2)$$

The eigenfunctions of the operator  $\mathbf{P}$  for a cold cavity device are the optical modes, and the corresponding eigenvalues  $\gamma$  determine the losses:  $\delta = 1 - |\gamma|^2$ .

An important issue in completing the definition of the eigenproblem is the necessity to impose the correct boundary conditions. While boundary conditions at the top and bottom of the construction are evident, this is not the case for lateral boundaries. Our particular interest is to explore the so-called leaky-wave modes. This requires that the radiation experience no reflection at the lateral boundaries. The only layer, which

has in-plane variable properties, is the spacer layer. The resonance wavelength shift in this layer according to [14] produces the required transverse index profile. Therefore, the absorbing boundary regions were added in this layer with proper extension of its sizes. The artificial absorption was introduced outside of each of the four lateral sides of the construction. The requirement that the artificial absorption has a negligible value in the region of the VCSEL design should be fulfilled. A particular care should be taken to avoid an influence of the absorption region on the wave-field reflection from the boundary. In selecting the amplitude and profile of the absorption function, we followed the authors [23].

The eigenproblem (2) can be solved in different ways. The first one is an analog of the Fox-Li iteration method by performing round-trips over the VCSEL. This approach allows us to find only one mode with the lowest losses. In the case for which the discrimination of modes is low, many iterations are required to converge on the fundamental mode. For the ARROW construction under consideration guided modes possess the lowest losses. Therefore, it is necessary to introduce an additional absorption into the ring-shaped waveguide to suppress the undesirable guided modes. In the actual VCSEL structure, absorbing QWs may be added to the spacer layers to accomplish this.

Another approach is to employ a method allowing for simultaneously computing an arbitrary number of modes. A sketch of the respective mathematical procedure is given below.

The operator  $\mathbf{P}$  acts in the complex space with a high dimension  $\mathcal{N} = N^2$  ( $N$  is the number of Fourier harmonics in wave-field decomposition for one Cartesian variable). In such a situation, a most appropriate way is to use Krylov's subspace methods for solving the eigenproblem. From practical considerations, only the few modes having the highest possible values of  $|\gamma|$  are of interest. Among known methods for treatment of the eigenproblem in the Krylov subspace, we utilize an Arnoldi algorithm [24] because of its simplicity and robustness properties.

In order to start the Arnoldi iterations, we have to determine an initial function  $\nu(x, y)$ . The appropriate way is to specify  $\nu = \mathbf{P}^K \psi$ , where  $\psi = \psi(x, y)$  is an arbitrary function, which can be considered as a seeded wave field, and  $K$  is the number of round trips, which this field made. Solutions to the eigenproblem (2) of interest to us are sought within the Krylov subspace

$$K_\Omega(\mathbf{P}, \nu) = \text{span}\{\nu, \mathbf{P}\nu, \mathbf{P}^2\nu, \dots, \mathbf{P}^{\Omega-1}\nu\}. \quad (3)$$

Physically, this means that the preliminary  $K$  iterations select such a wave-field distribution, which is composed of only modes with low losses. The number  $K$  of preliminary iterations and the Krylov subspace dimension  $\Omega$  are chosen empirically. Furthermore, the Gram–Schmidt orthogonalization technique is applied to create a basis in the Krylov subspace. Projection of the operator  $\mathbf{P}$  onto the Krylov subspace is realized by a Hessenberg matrix  $\mathbf{H}_\Omega$  of  $\Omega \times \Omega$  dimension. The eigenvalues  $\gamma_1, \gamma_2, \dots, \gamma_\Omega$  and eigenvectors  $h_1, h_2, \dots, h_\Omega$  of the matrix  $\mathbf{H}_\Omega$  can be calculated using any relevant standard program. The

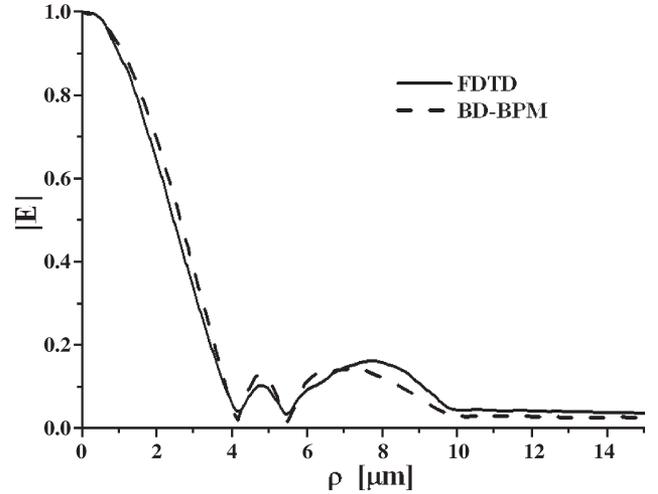


Fig. 2. Normalized amplitude of the electric field vector as a function of radial distance in the QW of an ARROW VCSEL with  $M = 2$  and  $s = 2 \mu\text{m}$ .

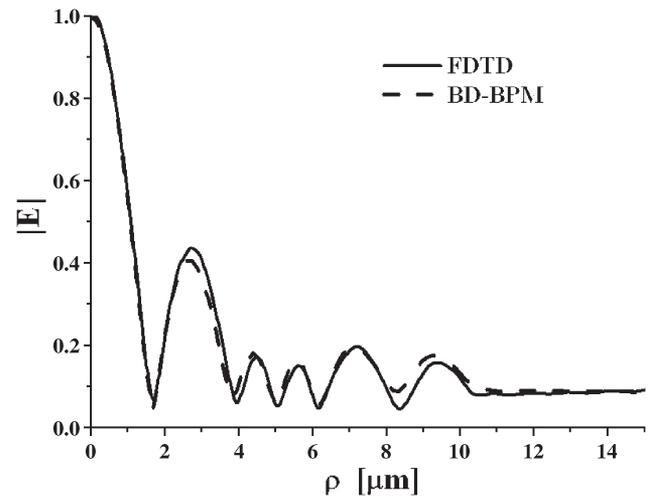


Fig. 3. Normalized amplitude of the electric field vector as a function of radial distance in the QW of an ARROW VCSEL with  $M = 2$  and  $s = 2 \mu\text{m}$ .

numbers  $\gamma_1, \gamma_2, \dots, \gamma_\Omega$  approximate the first  $\Omega$  eigenvalues of the round-trip operator  $\mathbf{P}$ . Approximate optical modes can then be expressed as linear combinations of vectors from the orthogonalized basis with eigenvectors  $\mathbf{H}_\Omega$  matrix weighting coefficients.

The small value of the optical mode loss sets a strict limit on the tolerances for an accuracy of a discrete approximation. The numerical scheme parameters were found from a condition of a sufficiently small loss change produced by increasing the accuracy of the calculations.

## V. COMPARISON OF RESULTS AND DISCUSSIONS

First, we consider the radial electric-field profiles of the cavity modes. The 3-D BD-BPM simulations of a specific VCSEL structure provide a set of modes ordered in terms of increasing loss. Each BPM-computed mode was identified after pairing it with the most similar FDTD-computed mode profile. Figs. 2–5 show comparisons of the normalized

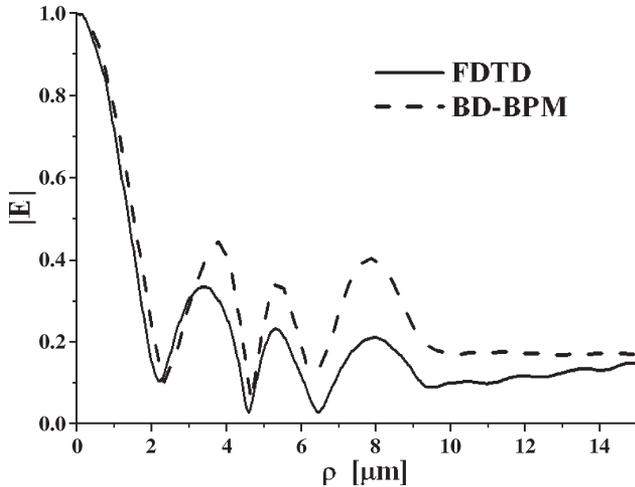


Fig. 4. Normalized amplitude of the electric field vector as a function of radial distance in the QW of an ARROW VCSEL with  $M = 3$  and  $s = 2 \mu\text{m}$ .

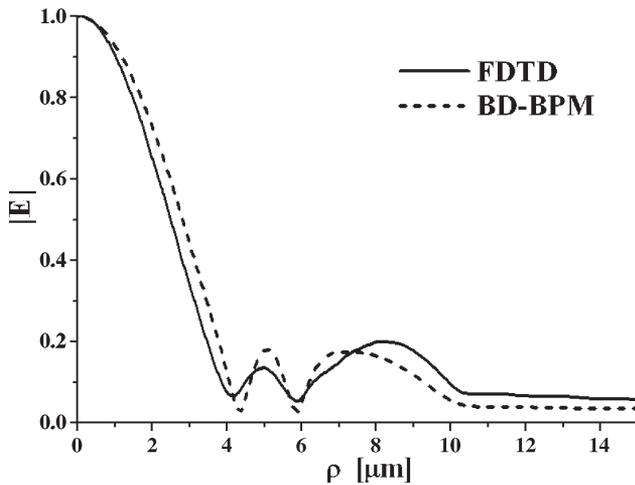


Fig. 5. Normalized amplitude of the electric field vector as a function of radial distance in the QW of an ARROW VCSEL with  $M = 3$  and  $s = 2 \mu\text{m}$ .

electric-field vector amplitudes of various modes as a function of radial distance in the active layer. In Figs. 2 and 3, the spacer layers, which generate the lateral index step, are located two  $p$ -DBR pairs away of the one-wavelength cavity (i.e.,  $M = 2$ ), the low-index core diameter is  $d = 8 \mu\text{m}$ , and the high-index reflector widths are  $s = 2$  and  $2.5 \mu\text{m}$ , respectively. In Figs. 4 and 5, the spacers are placed behind  $M = 3$   $p$ -DBR pairs (i.e., the lateral index step is lower). Since the index step is lower compared with the  $M = 2$  design, the width of the reflector at antiresonance (i.e., lowest loss) occurs at a larger value  $s = 2.5$ , compared with  $s = 2.0$  for the  $M = 2$  case. Figs. 2 and 5 illustrate the modal characteristics of the desired fundamental leaky mode. Figs. 3 and 4 show higher order leaky modes. As expected, these modes have much higher lateral-radiation losses; hence, their amplitudes in the outer part of the construction are remarkably greater. It is seen that the BD-BPM-computed mode profiles in Figs. 2, 3, and 5 agree quite closely with the FDTD-computed distributions. For

smaller  $s$  values, as shown in Fig. 4, the agreement between the two calculation methods is less quantitative.

Second, we consider the radiation losses of the fundamental mode. To compare results of the simulations by the two methods, we need to find a relation between  $Q$ -factors given by the FDTD method and modal losses calculated by the BD-BPM. The 3-D BD-BPM simulations demonstrated that in the absence of absorption in the spacer layers, leaky modes experience remarkably greater losses than the guided modes. Therefore, a special attention was paid to identify optical modes calculated in both methods.

The  $Q$ -factor is inversely proportional to the decay rate of a modal wave field in the cavity. This decay rate is determined by the round-trip duration and the fraction of the radiation lost in the course of this round-trip propagation. The duration of the round trip, in turn, is proportional to an effective cavity length. The authors of [25] suggested replacing a Bragg mirror in the paraxial approximation by a plane mirror placed at a certain distance behind the front of the Bragg mirror. Generally, reflection from the Bragg mirror results in the appearance of a phase advance proportional to the deviation from the exact resonance and leads to a modification to a spherical wavefront. As a whole, the VCSEL cavity can be modeled by the equivalent Fabry-Pérot cavity [26]. For our purposes, we need an equivalent length of the cavity  $L_C^{\delta k}$  arising from the dependence of the reflection coefficient of the Bragg mirror on frequency detuning from the resonance. For the particular axial configuration with a relatively low-index contrast in  $p$ - and  $n$ -Bragg gratings, a simplified expression for this length was derived in [19]

$$L_C^{\delta k} = [(1 - t_M)n_{2M}f_M + t_M(n_{2U}f_U + 2n_b) + 4n_i + n_{2L}f_L] \frac{\lambda}{4n_i^2}. \quad (4)$$

Here,  $f_j = (n_{1j}n_{2j})^{1/2}/(n_{2j} - n_{1j})$  is the inverse to Bragg grating contrast and  $j = U$  for upper  $p$ -DBR,  $j = L$  for bottom  $n$ -DBR,  $j = M$  for separating pairs of layers,  $t_M = \exp(-2Mf_M)$ ,  $n_i$  is the refractive index in the  $\lambda$ -cavity, and  $\lambda$  is the free-space resonant wavelength. Substituting respective values of the parameters for the constructions under study, one can find  $L_C^{\delta k}(M = 2) = 1.38\lambda$ , and  $L_C^{\delta k}(M = 3) = 1.35\lambda$ . The  $Q$ -factor can be expressed in terms of the mode eigenvalue  $\gamma$  as

$$Q = 2k_0n_i \frac{L_C^{\delta k}}{\delta} \quad (5)$$

$\delta = 1 - |\gamma|^2$ . It was found that for the fundamental mode (Figs. 2 and 5), the BD-BPM predicts losses 1.2–1.6 times higher than the FDTD simulations do. Generally, the discrepancy in losses found by two methods might be attributed to several sources: 1) an error introduced by the simplified expression (5) and 2) truncation of the angular spectrum of waves in the BD-BPM. For the ARROW construction with spacers behind two  $p$ -DBR pairs, both methods predict similar behavior of losses with respect to the mode order. For the

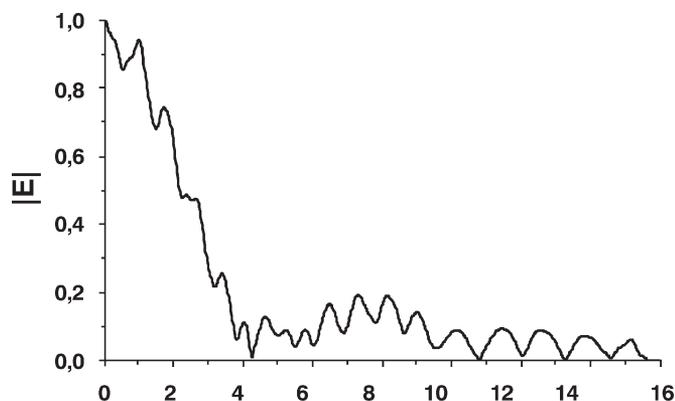


Fig. 6. FDTD-computed amplitude of the electric field vector as a function of radial distance at the top layer of an ARROW VCSEL with  $s = 2 \mu\text{m}$  and  $M = 2$ .

fundamental mode, the quantity  $10^4/Q$  as predicted by the FDTD method is 0.85, while by the BD-BPM, it is 1.07. For the higher order leaky mode shown in Fig. 3, the same quantity is 7.14 (FDTD) and 6.02 (BD-BPM), respectively. Thus, we find that within the framework of the approximations for the  $Q$ -factor computed by the BD-BPM, only relative comparisons of the modal dependence of  $Q$ -factor values are possible.

It is also of interest to examine the variation of the mode radial profile along the vertical axis. Fig. 6 shows the radial mode profile at the top layer of the structure found by the FDTD method. Comparing it with Fig. 3, the mode profile at the top layer exhibits similar behavior as in the active layer but with short-period ripples indicating an interference effect. The difference in field profiles in the active layer and at the top of the device found in FDTD simulations is probably the result of scattering of the mode wave field on the annular waveguide. The scattered waves propagate at a large angle without significant interaction with the Bragg layers and experience nearly total internal reflection (TIR) from the boundary GaAs/air. The amplitude of the modal field diminishes due to reflection from the Bragg mirror at least ten times and becomes comparable with the scattered field. Taking into account that a ripple period is close to the wavelength in vacuum, this explains their formation by interference of mode wave and oblique waves incident to the surface at the angle of TIR. Oblique waves reflecting from the GaAs/air boundary escape from the device through the bottom DBR and are absorbed in the uniaxial perfect matched layer (UPML). Therefore, one may neglect the influence of these waves on optical mode characteristics.

In contrast, BD-BPM predicts nearly identical mode profiles in the active layer and at the top layer (Fig. 7). This difference between the results of the simulations by the two methods can be explained by the fact that in the BD-BPM, the spatial frequency spectrum is truncated, leading to a smoothing of the fine structure in the mode profile. Good agreement in mode profiles calculated in the active layer by both methods confirms a negligible influence of oblique waves on optical mode formation.

The consideration of the cylindrical ARROW in frames of the EI-FMA theory [15] showed that a correct account of

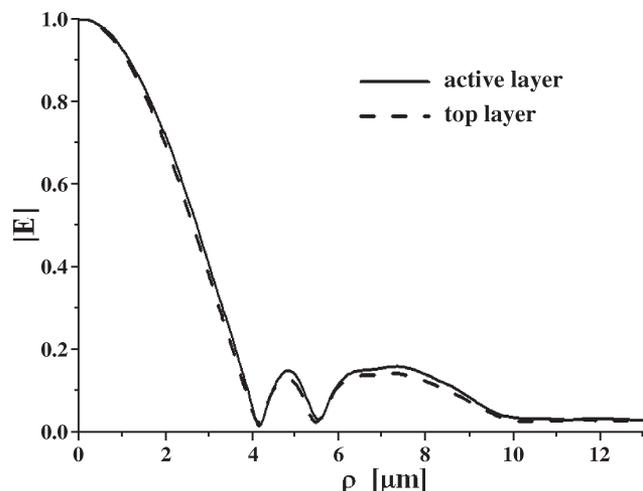


Fig. 7. BPM-computed amplitude of the electric field vector as a function of radial distance in an ARROW VCSEL with  $s = 2 \mu\text{m}$  and  $M = 2$ .

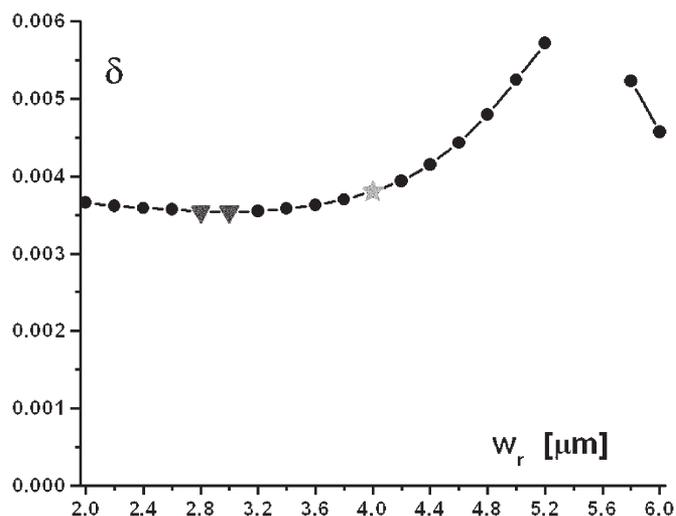


Fig. 8. Fundamental mode loss in dependence on the antiguided ring width for the construction  $s = 2 \mu\text{m}$  and  $M = 2$ , and  $d = 8 \mu\text{m}$ . Star designates the ring width  $d/2$ , which is optimal in the planar model, and triangles indicate the ring width corresponding to the minimum losses.

cylindrical geometry leads to a shift of antiresonance condition for the width of the (low-index) antiguided ring. We applied the BD-BPM to examine this prediction. The ARROW construction with  $d = 8 \mu\text{m}$ ,  $s = 2 \mu\text{m}$ ,  $M = 2$ , and variable antiguided ring width  $w_r$  was numerically studied. The calculated fundamental mode losses are displayed in Fig. 8 as a function of  $w_r$ . Indeed, in agreement with the EI-FMA theory [15], Fig. 8 shows that the fundamental mode has minimum losses for the construction where the antiguided ring width is in the range between 2.8 and 3  $\mu\text{m}$  instead of the value  $w_r = d/2 = 4 \mu\text{m}$  predicted by the theory in planar geometry.

## VI. CONCLUSION

A 3-D BD-BPM was developed to calculate the optical modes of VCSELS containing antiresonant optical waveguides.

The 3-D BD-BPM shows that the guided modes have the smallest losses in a cold cavity. A spectrum of guided and leaky modes was found for structures with a variable ring-shaped waveguide width and axial position. A number of leaky modes were calculated by the FDTD method. The radial profiles of leaky modes found by two approaches are compared, and an agreement between them is satisfactory. A tentative explanation is given of the discrepancies between modal losses calculated by two methods. The FDTD method predicts appearance of interference fringes in a mode profile at the last top layer of the device. This can be explained by the existence of waves totally reflected on the boundary top DBR air. The ARROW construction optimization was demonstrated by the 3-D BD-BPM. The external antiguided ring width giving minimum losses was found to be smaller than its value in the planar EI theory.

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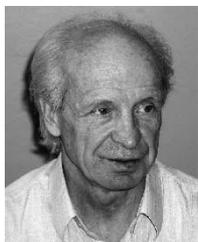
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