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Perfectly Matched Layers in Transmission Lines

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Abstract

The field distribution at the ports of the transmission line structure is computed by applying Maxwell's equations to the structure and solving an eigenvalue problem. The high dimensional sparse system matrix is complex in the presence of losses and Perfectly Matched Layer. A method is presented which preserves sparseness and delivers only the small number of interesting modes out with the smallest attenuation. The modes are found solving a sequence of eigenvalue problems of modified matrices with the aid of the invert mode of the Arnoldi iteration using shifts. A new strategy is described which allows the application of the method, first developed for microwave structures, to optoelectronic devices.

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1 Introduction

The design of microwave and optoelectronic devices requires efficient CAD tools in order to avoid costly and time-consuming redesign cycles. The fields of applications are mobile communications, radio links, automobile radar systems, optical communications and material processing. The commercial applications of microwave circuits cover the frequency range between 1 GHz and about 100 GHz, special applications in radioastronomy use even higher frequencies up to 1 THz. For optoelectronic devices frequencies about several hundred THz are common.
The structures under investigation can be described as an interconnection of infinitely long transmission lines, which have to be longitudinally homogeneous. Ports are defined on the transmission lines. The junction, the so-called discontinuity, may have an arbitrary structure. The whole structure must be surrounded with an enclosure.
For numerical treatment, the computational domain has to be truncated by electric or magnetic walls or by a so-called Absorbing Boundary Condition (ABC) simulating open space. Among the ABC's, the Perfectly Matched Layer (PML) [1] technique represents the most powerful formulation.
The field distribution at the ports can be calculated by applying Maxwell's equations to the transmission line structure and solving an eigenvalue problem [2]. The high dimensional sparse system matrix is complex in the presence of losses and PML.
First the method to find all eigen modes within in certain region of the complex plane was developed for microwave structures [3],[4]. The algorithm can also be applied to optoelectronic devices. The dimension and the number of eigenvalue problems to be solved increases essentially in this case caused by the high frequency. New strategies to handle these problems in a feasible time are described.

2 Boundary Value Problem

A three-dimensional boundary value problem can be formulated using the integral form of the Maxwellian equations in the frequency domain in order to compute the electromagnetic field:

$$\begin{aligned} \oint_{\partial\Omega} \vec{H} \cdot d\vec{s} &= \int_{\Omega} \jmath\omega[\epsilon]\vec{E} \cdot d\vec{\Omega}, & \oint_{\cup\Omega} ([\epsilon]\vec{E}) \cdot d\vec{\Omega} &= 0, \\ \oint_{\partial\Omega} \vec{E} \cdot d\vec{s} &= -\int_{\Omega} \jmath\omega[\mu]\vec{H} \cdot d\vec{\Omega}, & \oint_{\cup\Omega} ([\mu]\vec{H}) \cdot d\vec{\Omega} &= 0, \end{aligned} \tag{1}$$

$$\vec{D} = [\epsilon]\vec{E}, \quad \vec{B} = [\mu]\vec{H}. \tag{2}$$

At the ports p the transverse electric field $\vec{E}_t(z_p)$ is given by superposing transmission line modes $\vec{E}_{t,l}(z_p)$:

$$\vec{E}_t(z_p) = \sum_{l=1}^{m^{(p)}} w_l(z_p)\vec{E}_{t,l}(z_p). \tag{3}$$

The transverse electric mode fields have to be computed solving an eigenvalue problem for the transmission lines. All other parts of the surface of the computation domain are assumed to be an electric or a magnetic wall:

$$\vec{E} \times \vec{n} = 0 \quad \text{or} \quad \vec{H} \times \vec{n} = 0. \tag{4}$$

In order to simulate open structures we use Perfectly Matched Layers as an Absorbing Boundary Condition. The PML provide absorbing properties for any frequency, polarization and angle of incidence. These layers are filled with an artificial material with complex anisotropic material properties. Therefore, the complex permittivity $[\epsilon]$ and the complex permeability $[\mu]$ are diagonal tensors:

$$\begin{aligned} [\epsilon(x,y,z)] &= \epsilon_0 \ \mathrm{diag}\left(\tilde{\epsilon}_x + \frac{\tilde{\kappa}_e^x}{\jmath\omega}, \tilde{\epsilon}_y + \frac{\tilde{\kappa}_e^y}{\jmath\omega}, \tilde{\epsilon}_z + \frac{\tilde{\kappa}_e^z}{\jmath\omega}\right), \\ [\mu(x,y,z)] &= \mu_0 \ \mathrm{diag}\left(\tilde{\mu}_x + \frac{\tilde{\kappa}_m^x}{\jmath\omega}, \tilde{\mu}_y + \frac{\tilde{\kappa}_m^y}{\jmath\omega}, \tilde{\mu}_z + \frac{\tilde{\kappa}_m^z}{\jmath\omega}\right). \end{aligned} \tag{5}$$

The quantities ϵ_0 and μ_0 denote the permittivity and the permeability for a vacuum, $[\tilde{\epsilon}] = \mathrm{diag}(\tilde{\epsilon}_x, \tilde{\epsilon}_y, \tilde{\epsilon}_z)$ and $[\tilde{\mu}] = \mathrm{diag}(\tilde{\mu}_x, \tilde{\mu}_y, \tilde{\mu}_z)$ the relative permittivity and permeability, $[\kappa_e] = \epsilon_0 \ \mathrm{diag}(\tilde{\kappa}_e^x, \tilde{\kappa}_e^y, \tilde{\kappa}_e^z)$ and $[\kappa_m] = \epsilon_0 \ \mathrm{diag}(\tilde{\kappa}_m^x, \tilde{\kappa}_m^y, \tilde{\kappa}_m^z)$ the electric and magnetic (introduced for PML) conductivity, respectively. There is always an electric or magnetic wall (see (4)) behind the PML.

3 Maxwellian Grid Equations

The problem is solved numerically by the so-called Finite Difference Method in Frequency Domain (FDFD) (see [5]). Staggered nonequidistant rectangular grids are used. The electric field intensity components form a primary grid, and the magnetic flux density components a dual grid. Using a finite volume approach with lowest-order integration formulae

$$\oint_{\partial\Omega} \vec{f} \cdot d\vec{s} \approx \sum(\pm f_i s_i), \qquad \int_{\Omega} \vec{f} \cdot d\vec{\Omega} \approx f\Omega \tag{6}$$

Maxwell's equations are transformed into a set of Maxwellian grid equations:

$$\begin{aligned} A^T D_{s/\tilde{\mu}} \vec{b} &= \jmath\omega\epsilon_0\mu_0 D_{A_{\tilde{\epsilon}}} \vec{e}, & B D_{A_{\tilde{\epsilon}}} \vec{e} &= 0, \\ A D_s \vec{e} &= -\jmath\omega D_{A_{\tilde{\mu}}} \vec{b}, & \tilde{B} D_{A_{\tilde{\mu}}} \vec{b} &= 0. \end{aligned} \tag{7}$$

The vectors $\vec{e}$ and $\vec{b}$ contain the components of the electric field intensity $\vec{E}$ and of the magnetic flux density $\vec{H}$ of the elementary cells, respectively. The diagonal matrices

$D_{s/\tilde{\mu}}$, $D_{A_{\tilde{\epsilon}}}$, D_s, and $D_{A_{\tilde{\mu}}}$ contain the information on cell dimension and material. A, B and $\tilde{B}$ are sparse and contain the values 1, -1 and 0 only. Substituting the components of the magnetic flux density from the two equations of the left-hand sides of (7) the number of unknowns can be reduced by a factor of two and we get the system of linear algebraic equations

$$(A^T D_{s/\tilde{\mu}} D^{-1}_{A_{\tilde{\mu}}} A D_s - k_0^2 D_{A_{\tilde{\epsilon}}})\vec{e} = 0, \quad k_0 = \omega\sqrt{\epsilon_0 \mu_0}, \tag{8}$$

which has to be solved using the boundary conditions. k_0 is the wavenumber in vacuum.

4 Eigen Mode Problem

Because the transmission lines are longitudinally homogeneous any field can be expanded into a sum of modal fields which vary exponentially in the longitudinal direction:

$$\vec{E}(x, y, z \pm 2h) = \underline{\vec{E}}(x, y, k_z) e^{\mp \jmath k_z 2h}. \tag{9}$$

A substitution of this ansatz into the system of linear equations (8) and the elimination of the longitudinal electric field intensity components by means of the electric-field divergence equation (see equations (7)) gives an eigenvalue problem:

$$C\underline{\vec{e}} = \gamma \underline{\vec{e}}, \quad \gamma = -4\sin^2(hk_z). \tag{10}$$

$\underline{\vec{e}}$ consists of components of the discretized eigenfunctions $\underline{\vec{E}}$. $2h$ is the length of an elementary cell in z-direction. The relation between the eigenvalues γ and the propagation constants k_z is nonlinear:

$$k_z = \frac{\jmath}{2h} \ln\left(\frac{\gamma}{2} + 1 + \sqrt{\frac{\gamma}{2}\left(\frac{\gamma}{2} + 2\right)}\right) = \beta - \jmath\alpha. \tag{11}$$

We are interested only in a few modes with the smallest attenuation. These are the modes with the smallest magnitude of imaginary part, but possibly with large real part of their propagation constant. The computation of all eigenvalues in order to find a few propagation constants must be avoided for the high-dimensional problem. For numerical treatment we have to limit the search for propagation constants by a maximum value k_f of their real part. For the propagation constant k_z of a waveguide homogeneously filled with isotropic material with the permittivity ϵ and the permeability μ we have

$$\Re(k_z) \leq \Re(k), \quad \text{with} \quad k = \omega\sqrt{\epsilon\mu}. \tag{12}$$

k is the wavenumber of a plane wave in the same material. From this, we assume that for inhomogeneously filled waveguides the relation

$$\Re(k_z) \leq k_f = \omega\Re(\sqrt{\epsilon_l \mu_l}) \tag{13}$$

holds, where ϵ_l and μ_l are properties of the material that yields the largest value of the right-hand side of Equation (13) (see also [6]). Modes with fields concentrated in metals would be strongly attenuated. As we are interested in propagating modes, we can exclude all metals from the search for ϵ_l and μ_l. The PML's can also be excluded from the search for ϵ_l and μ_l, since propagating modes are concentrated in the area of the waveguide.
Using k_f from (13) and a preset maximum value α_m of the imaginary part of the propagation constants the region containing the interesting constants is defined as a rectangle $\hat{F}$ (see Figure 2) bounded by the lines

$$\beta = \pm k_f \quad \text{and} \quad \alpha = \alpha_m. \tag{14}$$

We can use the approximation $\sin(x) \approx x$ in (10) if we choose h to be small enough, which is necessary anyway to get small discretization errors:

$$\gamma = -4\sin^2(hk_z) \approx -4(hk_z)^2 = u + \jmath v. \tag{15}$$

With aid of the approximation (15) we get a conformal mapping between the plane of eigenvalues (γ-plane) and the plane of propagation constants (k_z-plane, see (11)):

$$u = -4h^2(\beta^2 - \alpha^2), \quad v = 8h^2\alpha\beta. \tag{16}$$

Using this mapping the rectangle $\hat{F}$ of the k_z-plane is transformed into a region F of the γ-plane bounded by the two parabolas

$$v = \pm 4hk_f\sqrt{u + 4h^2{k_f}^2} \quad \text{and} \quad v = \pm 4h\alpha_m\sqrt{-u + 4h^2{\alpha_m}^2}. \tag{17}$$

That means, we have to find all eigenvalues of the region bounded by the parabolas (see Figure 1).

5 Computation of Eigen Modes

The dimension n of the eigenvalue problem (10) is too large to use a direct method. We need an algorithm that computes just a few selected eigenvalues and eigenvectors of a complex sparse matrix. A state-of-the-art algorithm for such problems is the Arnoldi method [7], [8]. In general the Arnoldi method converges for our problem only using the invert mode and looking for eigenvalues of largest magnitude. Thus, a simple way to find the eigenvalues located in the region F would be to look for all eigenvalues of smallest magnitude, which are located in a circle centered on the origin and covering the region F. Caused by the high wavenumber k_f, the number of eigenvalues located in this circle is too much in general for a feasible computation using an iterative method. We can solve this problem covering the region F with $s \geq 1$ circles C_i, $i = 1(1)s$, centered on the u-axis and calculating the eigenvalues located in these circles. That is done in the following way. s points $\hat{P}_i(\beta_i, \alpha_m)$ with

$$\beta_i = i\frac{k_f}{s}, \quad \text{if} \quad \frac{k_f}{s} \geq \bar{\beta}, \quad s \quad \text{given}, \quad \bar{\beta} = \sqrt{3}\alpha_m, \quad i = 1(1)s, \tag{18}$$

are calculated on the interval $[0, k_f]$ of the line $\alpha = \alpha_m$. The meaning of the minimum distance $\bar{\beta}$ is discussed below. The number s and the location of the points P_i can be changed by the method described below. In this case we could have $\beta_s > k_f$ in order to fulfill condition $\frac{k_f}{s} \geq \bar{\beta}_s$. The points $\hat{P}_i$ are transformed into the points $P_i(u_i, v_i)$ of the γ-plane using (16). They are located on the parabola ((17), right formula). s circles C_i centered on the u-axis are built with the points P_i:

$$(u + m_i)^2 + v^2 = {r_i}^2, \;\; r_i = \sqrt{(\Im(P_i))^2 + (m_i - \Re(P_i))^2}, \quad i = 1(1)s, \tag{19}$$

with

$$m_1 = 0, \;\; m_i = \frac{(\Re(P_{i+1}))^2 - (\Re(P_i))^2 + (\Im(P_{i+1}))^2 - (\Im(P_i))^2}{\Re(P_{i+1}) - \Re(P_i)}. \tag{20}$$

The circles C_i cover the region bounded by the parabolas (17) (see Figure 1).
In order to find all eigenvalues, located in the circle C_i, l points Q_j are defined on the periphery of C_i. The matrix C is extended by the diagonal matrix Q. The diagonal elements of Q are the l complex elements Q_j:

$$\bar{C} = \begin{pmatrix} Q & \\ & C \end{pmatrix}, \quad Q = diag(Q_1, ..., Q_l). \tag{21}$$

The s eigenvalue problems

$$(\bar{C} - m_i I)\underline{\vec{e}} = (\gamma - m_i)\underline{\vec{e}}, \quad i = 1(1)s, \tag{22}$$

are solved with the aid of the implicitly restarted Arnoldi method using the invert mode. The eigenvalue problems can be solved separably. We consider one circle C_i. The number m of eigenvalues to be computed for this circle must be l on the first call to the Arnoldi procedure. The main idea is to raise m by l for so long until at least one value Q_j was found. But, since $m \ll n$ (n order of matrix $\bar{C}$) for a feasible computation, one has to restrict the number m of required eigenvalues by m_{max}. If m exceeds m_{max} we look for the eigenvalue γ_{max} of largest magnitude located in circle C_i. If

$$|\Im(P_i)| < \sqrt{|\gamma_{max}|} \tag{23}$$

we define a new circle $\tilde{C}_i$ of radius $\sqrt{|\gamma_{max}|}$ centered on the u-axis and containing P_i on the periphery. May be $\tilde{P}_{i+1}$ the intersection point of $\tilde{C}_i$ with the parabola ((17), right formula). The distance between the corresponding points in the k_z-plane is

$$\Delta\hat{\tilde{P}} = \Re(\hat{\tilde{P}})_{i+1} - \Re(\hat{P}_i). \tag{24}$$

If $\Delta\hat{\tilde{P}} \geq \bar{\beta}$ (see (18)) we accept the new circle and proceed with the distance $\Delta\hat{\tilde{P}}$. We insert a point $\hat{P}_{i+\frac{1}{2}}$ between $\hat{P}_i$ and $\hat{P}_{i+1}$, if condition (23) or $\Delta\hat{\tilde{P}} \geq \bar{\beta}$ is not fulfilled. That means, two eigenvalue problems have to be solved for the interval $[\hat{P}_i, \hat{P}_{i+1}]$ rather than one. This procedure can be repeated taking into account that the minimum distance $\Delta\hat{P}$ between two neighboring points should not be fall below $\bar{\beta}$. The same procedure is used if a given number ν_{max} of iterations in the Arnoldi

method is exceeded.
Separating the new values on each eigenvalue problem i, we are sure to have found all eigenvalues which are located in the corresponding circles C_i. The number m of eigenvalues to be computed for the circle C_{i+1} is adapted to the number of eigenvalues found in C_i.
Applying the mapping (16) the circles C_i (see (19)) are transformed into Cassinian curves $\hat{C}_i$

$$(\beta^2 + \alpha^2)^2 - \frac{m_i}{2h^2}(\beta^2 - \alpha^2) = \frac{{r_i}^2}{16h^4} - \frac{{m_i}^2}{16h^4}, \tag{25}$$

which cover the rectangle $\hat{F}$ containing all desired propagation constants. Propagation constants outside of $\hat{F}$ and PML-Modes (see Section 6) are eliminated. The Cassinian curves $\hat{C}_i,\ \ i = 2(1)s$, consist of two separated ovals (see Figure 2, right and left curve), if $r_i < m_i$. Using $\bar{\beta}$ as minimum distance between two points $\hat{P}_i$ and $\hat{P}_{i+1}$ (see (18)) other shapes of Cassinian curves (e.g. waisted oval in Figure 2), which would lead to higher execution times, are avoided.
If the condition $\Delta\hat{P} \geq \bar{\beta}$ cannot be fulfilled, we have to restart with new parameters m_{max}, ν_{max} and possibly α_m.
Because in general the Arnoldi method does not converge using the regular mode for our eigenvalue problem the invert mode with shifting (see (22)) is applied. A system of linear algebraic equations has to be solved on each iteration step in this case. We use the combined unifrontal/multifrontal method [9] for the solution of the partly ill-conditioned nonsymmetric complex linear algebraic equations.

6 Detection of PML Modes

The PML is applied in order to compute the eigen modes of open waveguide structures. Introducing the PML permits the calculation of radiation effects. Additionally the absorbing boundary suppresses the interaction between the waveguide modes and higher order modes, caused by the finite simulation domain. Anyway, these undesired modes are generated, due to the electric or magnetic walls behind these absorbing boundary layers. The PML shifts these box modes inside the $\hat{F}$ area. As a criterion to distinguish between waveguide modes and undesired modes we use the power concentration of all modes by way of comparison. Undesired modes are characterized by a high power concentration inside the PML region, while propagating modes are concentrated in the waveguide area. Thus, to eliminate the PML-modes we calculate the magnitude of the power flow of each computed mode in the PML ($P^{(P)}$), in the waveguide region ($P^{(W)}$), and in the total computational domain (P):

$$P = P^{(P)} + P^{(W)} = \int\limits_{\Omega^{(P)}} \left(\vec{E}_t \times \vec{H}^*_{t,m}\right) \cdot d\vec{\Omega} + \int\limits_{\Omega^{(W)}} \left(\vec{E}_t \times \vec{H}^*_{t,m}\right) \cdot d\vec{\Omega}\,. \tag{26}$$

A mode is specified as PML-mode if the ratio

$$r^{(P)} = \frac{P^{(P)}}{P} > \xi\,, \tag{27}$$

with values $\xi = 0.2, \dots, 0.6$, found empirically, is satisfied.

7 Application

As an example we have calculated the guided mode of an optoelectronic device. A so called self aligned stripe (SAS) laser is investigated, see Figure 3. This laser structure contains an additional, so called antiguided layer (marked with yellow color in Figure 3) outside the emitting stripe (marked with red color in Figure 3). This high power laser diode excites only the fundamental mode, the active region is useful for wavelengths shorter than 800 nm. In our eigen mode computation of the laser structure a graded mesh of 211 times 322 elementary cells, including 10-cell PML regions, is used. The frequency is fixed to $299.7925 * 10^{12}$ Hz. The maximum cell size amounts $\frac{\lambda}{12} = 25\,\mathrm{nm}$, where λ denotes the wavelength in the material with the highest $\Re(\epsilon)$. The minimum cell size is 3 nm. Maximum cell size is scaled down exponentially in the vertical direction near the 100 nm zones and in the horizontal direction near the material cut 107 and 108 (see Figure 3). The dimension of the eigenvalue problem is approximately 135 000. 74 Cassinian curves have been used to cover the long small region of the complex plane ($\alpha_m = 2500\,\mathrm{m}^{-1}$, $k_f = 21765592.37\,\mathrm{m}^{-1}$, see (14) and Figure 4) containing potential guided modes. The long small region is caused by the high wavenumber. One guided mode according to the lasers fundamental mode, was found. The computed complex propagation constant is given by

$$\epsilon_{\mathrm{eff}} = \left(\frac{k_z}{k_0}\right)^2 = 10.978012 + \jmath 0.001545, \;\; k_0 = 2\frac{\pi}{\lambda_0}, \tag{28}$$

λ_0 denotes the wavelength in vacuum. k_0 is designed with ak0 in Figure 4.

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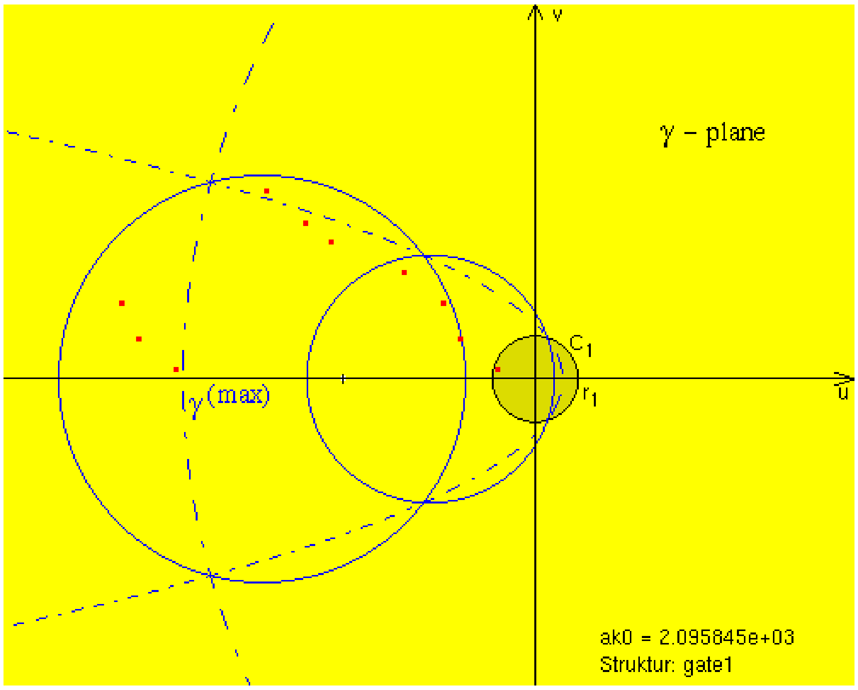

Figure 1: γ-plane, coplanar waveguide

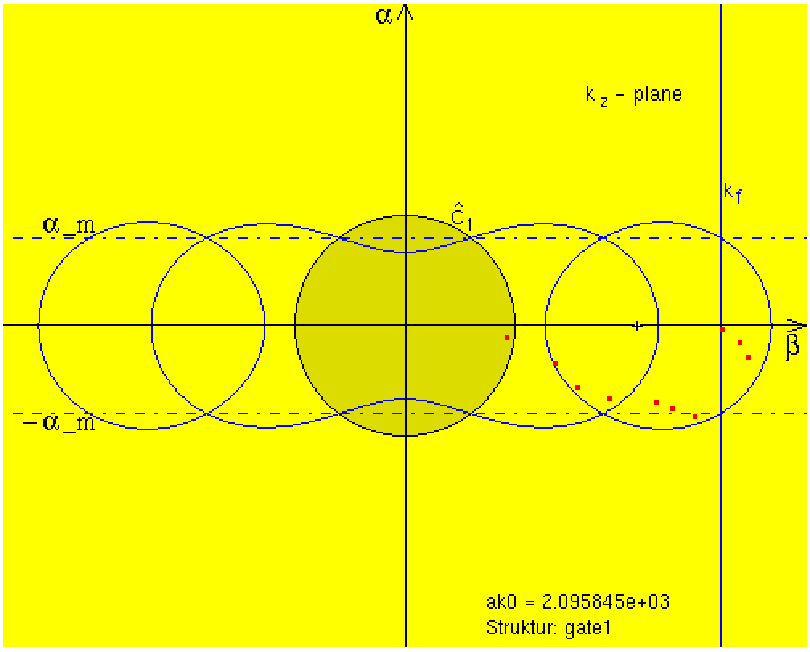

Figure 2: k_z-plane, coplanar waveguide

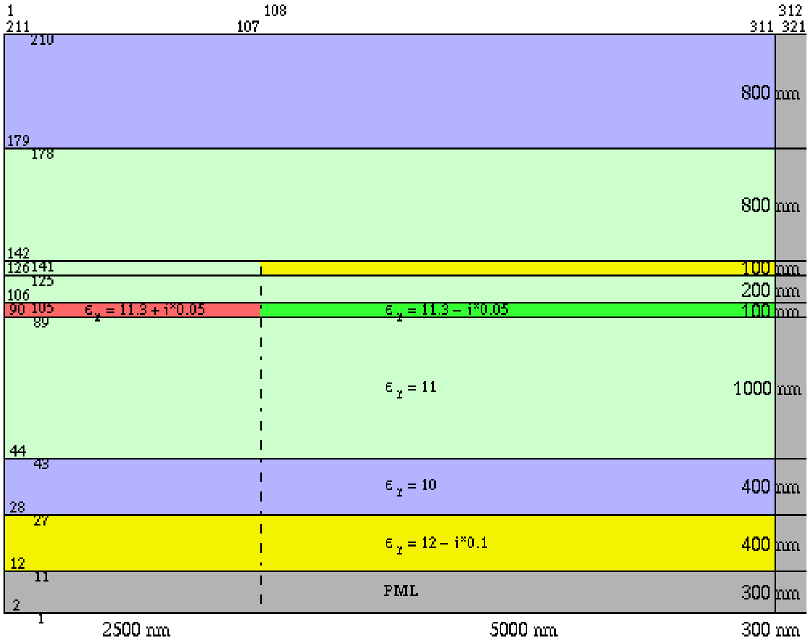

Figure 3: Laser (amplifier)

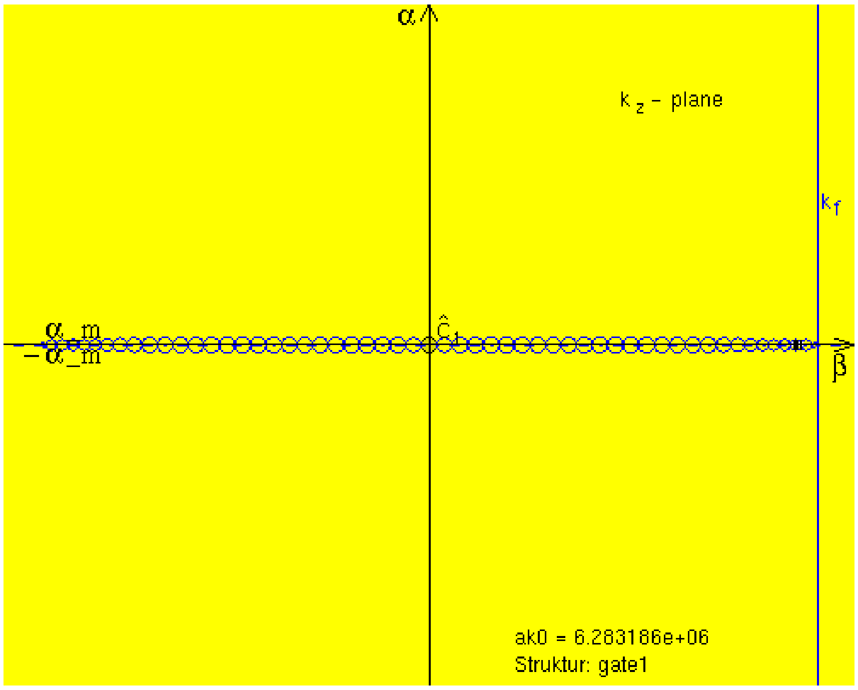

Figure 4: kz-plane, Laser

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