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High-Order Finite-Element Analysis of Scattering Properties of II-VI Semiconductor Materials

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The scattering characteristics of the II-VI semiconductors were analyzed by a method which combines the second-order finite-element method with the rigorous mode matching procedure. The method avoids the difficulty of solving the complex transcendental equation introduced in the multimode network method and calculates all the eigenvalues and eigenfunctions simultaneously which are needed for the mode matching treatment in the longitudinal direction. As a result, the whole solution procedure is significantly simplified. A comparison is given between the experimental data and the calculated results obtained with this analysis and the network method. Very good agreement has been achieved, the accuracy and efficiency of the present method are thus verified.

KEYWORDS: II-VI semiconductor, scattering characteristics, high-order finite-element, mode matching method.

I. INTRODUCTION

Recently, II-VI semiconductors have become increasingly important in material science and

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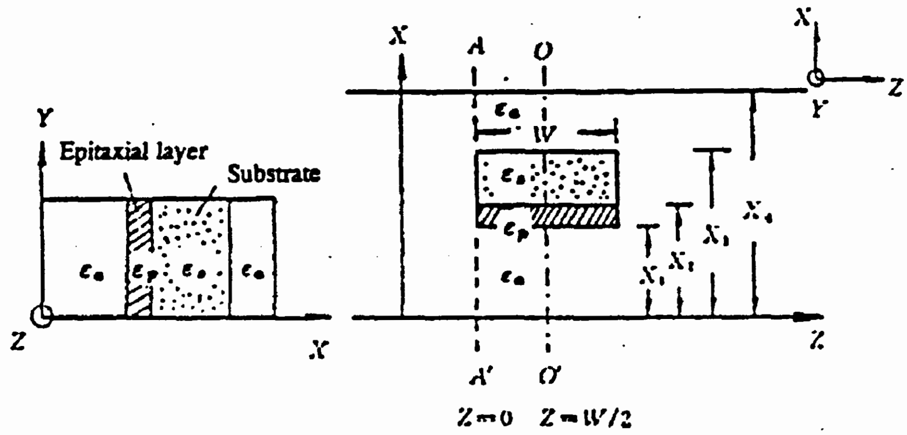

Fig. 1
Scheme of a discontinuity structure formed by semiconductor sample.

engineering because of their inherent advantages for applications in optoelectronic, infrared and millimeter wave techniques. For these purposes, the exact knowledge of their electric properties, e.g., conductivity, is of essential significance. However, poorly conducting II-VI semiconductors have always created problems. In many cases, it is extremely difficult or even impossible to obtain good ohmic contacts to the sample. For characterizing II-VI compounds under these circumstances, a contactless conductivity measurement [1] has been developed employing a microwave bridge technique. The basic idea of this method is that the determination of property parameters of a semiconductor sample is transferred to the measurement of the scattering characteristics of the corresponding sample. The key point of realizing this idea is to determine theoretically the relationship between the property parameters of the semiconductor and scattering parameters of the corresponding sample. This is a complex boundary problem of electromagnetic field. The complexity of the problem consists of the following two aspects.

1) The conductivity of the epitaxial layer may vary in a wide range from several tens to some thousands (mho/cm) to satisfy the practical requirements of different devices. As a result, the real and imaginary parts of the corresponding complex dielectric constants may be very large; in particular, the imaginary part may vary from several hundreds to some millions. If the calculating method is not chosen properly, it may suffer from a convergence problem. In addition, because the epitaxial layer is neither an ideal dielectric nor ideal conductor, some assumptions for these two extreme circumstances cannot be used; for instance, one cannot simplify the problem with approximate methods such as perturbation theory.

2) Although the epitaxial layer is very thin (only 1 to 5 μm, or even less than 1 μm), it cannot be assumed to be zero. Investigating the effect of the thickness on scattering characteristics is one of the tasks of this paper. Therefore, it may also cause a convergence problem if the method is not correctly adopted. The problem was solved by a method which combined the multimode network theory with rigorous mode matching procedure [2]. However, in this method, the analysis of the eigenvalue problem of the waveguide is transferred to the solution of the complex transcendental equation. To accurately calculate more than twenty roots of this equation consecutively without missing one root, it is needed to search for the roots many times. Obviously, this is time-consuming. In particular, this is a very difficult job for those who have little experience in seeking roots for the complex transcendental equation.

Alternatively, the problem is solved in this article by a method which combines the finite element method with the rigorous mode matching procedure. The method not only avoids the difficulty of

Table 1
Parameters of different semiconductor samples.

Sample	ϵ_s	ϵ_p	d_s (mm)	d_p (μm)
CMT78 (HgCdTe)	11.–j0.8	–41.–j1816	1.0	2.0
CMT76(HgTe)	11.–j0.45	–198.–j7779	1.0	1.2
Q154 (HgCdTe)	11.–j0.5	–358.–j13538	1.0	2.2
Q114 (HgCdTe)	11.–j0.5	–2861.–j103052	1.0	5.2
Q107 (HgCdTe)	11.–j11	–6254.–j223684	1.0	2.9
Q105 (HgCdTe)	11.–j0.5	–8285.–j296801	1.0	1.6

solving the complex transcendental equation, but calculates all the eigenvalues and eigenfunctions simultaneously needed for the mode matching treatment in the longitudinal direction, so the procedure is greatly simplified, and the efficiency of calculations is increased. A comparison is given between the experimental data and the calculated results obtained with this analysis and the network method. Very good agreement has been achieved, and the accuracy and efficiency of the method are thus verified.

II. METHOD OF ANALYSIS

Figure 1 shows the cross section of the stratified dielectric discontinuity structure under consideration. Here the dielectric constants of the epitaxial layer and the substrate are complex with real and imaginary parts. Table 1 shows the thicknesses and the dielectric constants of the epitaxial layers and the substrates for several samples. For our semiconductor samples we assume the relative permeability $\mu = 1$, thus excluding semimagnetic samples. In the standard rectangular waveguide, the dominant mode is the TE_{10} mode, of which the fields are invariant in the y-direction. Since the discontinuity is uniform in the same direction both in geometrical dimensions and in dielectric distributions, only the TE_{m0} mode can be excited in the empty and in the partially filled waveguides. Therefore, the scattering problem is two dimensional. The solution procedure for this problem may be divided into two steps.

1) We must analyze the eigenvalue problem of the two waveguides, respectively, in the transverse cross section.

2) We must calculate the scattering characteristics of the discontinuity in the longitudinal cross section.

As the eigenvalues and the eigenfunctions for the empty waveguide are well known, the key point to the eigenvalue problem in the first step is the determination of the eigenvalues and the eigenfunctions in the partially filled waveguide. According to the fact that only TE_{m0} mode is excited, a one-dimensional functional formulation is derived, and the corresponding variational problem is solved with the finite-element method.

It is well known that the eigenfunctions and eigenvalues of TE_{m0} modes in the empty rectangular waveguide are, respectively, as follows, omitting phase factors like $\exp[j(\omega t - K_{zm}z)]$:

$$\varphi_m = A_m \sin(K_{xm} X), \tag{1}$$

$$K_{xm} = m\pi / X_4, \tag{2}$$

$$K_{zm}^2 = K_0^2 - K_{xm}^2; \tag{3}$$

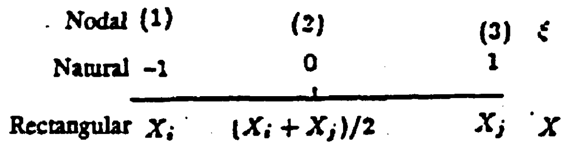

Fig. 2
Coordinate relation in the second order line element.

where K_0 is the free space wavenumber and the amplitude of the m-th eigenmode is A_m, which can be obtained, with the orthonormal relation, as:

$$A_m = \sqrt{2/X_4}; \tag{4}$$

The transverse electromagnetic fields in the empty waveguide may be expressed in terms of the superposition of the complete set of the eigenmode functions as:

$$E_y = \sum_m^{\infty} V_m \varphi_m, \tag{5}$$

$$H_x = \sum_m^{\infty} I_m \varphi_m. \tag{6}$$

It is easy to derive that the electric field E_y of each H_{m0} modes in the partially filled waveguide satisfies the following ordinary differential equation:

$$\frac{d^2 E_y}{dx^2} + (K_0^2 \varepsilon_r(x) - K_z^2) E_y = 0, \tag{7}$$

where $\varepsilon_r(x)$ is uniform in each segment, i.e., ε_a, ε_p, ε_s and ε_w for their respective different segments. as shown in Fig. 1.

It has been proved that the above complex eigenvalue problem is equivalent to the variational problem of the following functional:

$$F(E_y) = \int_l \left[\left(\frac{dE_y}{dx} \right)^2 - (K_0^2 \varepsilon_r - K_z^2) E_y^2 \right] dx. \tag{8}$$

When the finite-element method is applied to solve the above-mentioned variational problem, the unknown function in each element is interpolated from the nodal parameters. Here the second-order finite-element method is used. Therefore, the function E_y in each element can be expressed as:

$$E_y^e = \sum_{i=1}^{3} N_i(\xi) E_{yi}^e = (N)^T (E_y^e); \tag{9}$$

with

$$N_1(\xi) = \frac{1}{2}\xi(\xi - 1), \tag{10}$$

$$N_2(\xi) = 1 - \xi^2, \tag{11}$$

$$N_3(\xi) = \frac{1}{2}\xi(\xi + 1), \tag{12}$$

$$\xi = \frac{2}{x_j - x_i}\left(x - \frac{x_i + x_j}{2}\right). \tag{13}$$

According to the variational principle, substituting Eqs. (9) into (8), we obtain the following eigenvalue problem:

$$[A](E_y) - K_0^2[C](E_y) + K_z^2[B](E_y) = 0. \tag{14}$$

Equation (14) can be written as the following generalized algebraic eigenvalue equation:

$$[D](E_y) = K_z^2[B](E_y); \tag{15}$$

with

$$[A] = \sum_e \int_e (N_x)(N_x)^T \mathrm{d}x, \tag{16}$$

$$[B] = \sum_e \int_e (N)(N)^T \mathrm{d}x, \tag{17}$$

$$[C] = \sum_e \varepsilon_r \int_e (N)(N)^T \mathrm{d}x; \tag{18}$$

$$[D] = K_0^2[C] - [A], \tag{19}$$

where $(N_x) = \partial(N)/\partial x$. The integrals in Eqs. (17), (18), (19) are calculated by:

$$\int_e (N_x)(N_x)^T \mathrm{d}x = \frac{1}{3(x_j - x_i)}\begin{bmatrix} 7 & -8 & 1 \\ -8 & 16 & -8 \\ 1 & -8 & 7 \end{bmatrix}, \tag{20}$$

$$\int_e (N)(N)^T \mathrm{d}x = \frac{(x_j - x_i)}{30}\begin{bmatrix} 4 & 2 & -1 \\ 2 & 16 & 2 \\ -1 & 2 & 4 \end{bmatrix}. \tag{21}$$

From the generalized algebraic eigenvalue equation, the eigenvalue K_z of the H_{m0} modes and corresponding eigenvector (E_y) are obtained, and the nth eigenfunction in a partially filled waveguide can be expressed as:

$$\bar{\varphi}_n = \overline{A}_n \sum_e \sum_{i=1}^{3} N_i^e \overline{E}_{yni}^e; \tag{22}$$

where E_{yni}^e is the i-th nodal value in the e-th element for the eigenvector (E_{yn}). The amplitude A_n of the n-th eigenmode can be obtained with the orthonormal relation:

$$\int_0^{x_4} \overline{\varphi}_n^2 \mathrm{d}x = 1. \tag{23}$$

Also, the transverse electromagnetic fields in the partially filled waveguide may be expressed in terms of the superposition of the complete set of the eigenmode functions as:

$$\overline{E}_y = \sum_n^{\infty} \overline{V}_n \overline{\varphi}_n, \tag{24}$$

$$\overline{H}_x = \sum_n^{\infty} \overline{I}_n \overline{\varphi}_n. \tag{25}$$

At the discontinuity interface plane *A-A'* ($z = 0$), the tangential fields E_y and H_x must be continuous, i.e.,

$$E_y = \overline{E}_y, \tag{26}$$

$$H_x = \overline{H}_x; \tag{27}$$

or

$$\sum_m^{\infty} V_m \varphi_m = \sum_n^{\infty} \overline{V}_n \overline{\varphi}_n, \tag{28}$$

$$\sum_m^{\infty} I_m \varphi_m = \sum_n^{\infty} \overline{I}_n \overline{\varphi}_n. \tag{29}$$

These equations hold for any x in the $z = 0$ plane. By scaler multiplication of these equations with either φ_n or $\bar{\varphi}_m$ and making use of the orthonormal relation:

$$\int_0^{x_4} \varphi_m \varphi_n \mathrm{d}x = \delta_{mn}, \tag{30}$$

$$\int_0^{x_4} \overline{\varphi}_m \overline{\varphi}_n \mathrm{d}x = \delta_{mn}; \tag{31}$$

we then have

$$(V) = [Q](\overline{V}), \tag{32}$$

$$(I) = [Q](\overline{I}); \tag{33}$$

where (V), (I), $(\bar{V})$ and $(\bar{I})$ are the column voltage and current vectors formed by the factors V_m, I_m, $\bar{V}_n$ and $\bar{I}_n$, respectively, representing the amplitudes of the electric field E_y and the magnetic field H_x outside and inside the discontinuity region. $[Q]$ is the coupling matrix, its typical element Q_{mn} is given by

$$Q_{mn} = \int_0^{x_4} \varphi_m \overline{\varphi}_n \mathrm{d}x. \tag{34}$$

It can be proved that

$$[Q][Q]_t = E; \tag{35}$$

where "t" stands for "transpose" and E is the unit matrix. According to the definition of the impedance of a multimode network, we have

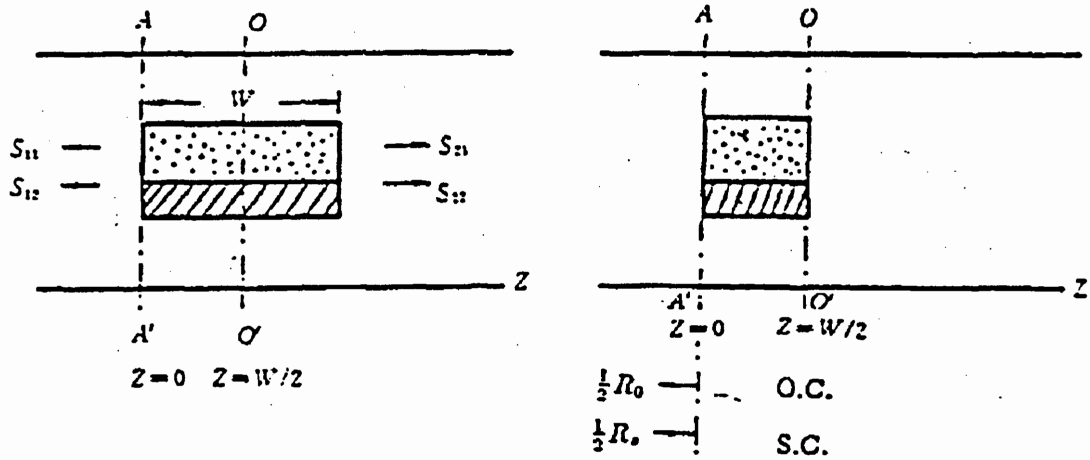

Fig. 3
Symmetrical consideration of the structure in the longitudinal direction.

$$(V) = [Z](I), \tag{36}$$

$$(\overline{V}) = [\overline{Z}](\overline{I}); \tag{37}$$

and then we can obtain the relation

$$[Z] = [Q][\overline{Z}][Q]_t; \tag{38}$$

where $[Z]$ and $[\tilde{Z}]$ are, respectively, the input impedance on two sides of the discontinuity plane A-A' ($z = 0$). This is actually an impedance transformation formula from which the reflection coefficient of each guide mode at $z = 0$ plane can be determined [3-5].

It is worthwhile to note that the present structure is symmetrical in the longitudinal cross section as shown in Fig. 3. The scattering of a guided mode by such a symmetrical structure may be analyzed in terms of the symmetrical and anti-symmetrical excitations for which we have the open-circuit (O.C.) and short-circuit (S.C.) bisections, respectively, as indicated in Fig. 2.

The reflection coefficient for each guide mode at the symmetry plane $z = W/2$ (O-O' plane) is 1.0 for the O.C. bisection or -1.0 for the S.C. bisection. Let $[R_0]$ and $[R_s]$ be the reflection coefficient matrices at $z = 0$ plane for the O.C. and the S.C. bisections, respectively; the guided mode reflection coefficient matrix [R] (at $z = 0$ plane) and the transmission matrix $[T]$ (at $z = W$ plane) of the entire symmetrical structure are then given by:

$$[R] = ([R_0] + [R_s])/2, \tag{39}$$

$$[T] = ([R_0] - [R_s])/2; \tag{40}$$

where $[R_0]$, $[R_s]$ can be obtained from the following formulas:

$$[R_0] = ([Z_0] + [Z_c])^{-1}([Z_0] - [Z_c]), \tag{41}$$

$$[R_s] = ([Z_s] + [Z_c])^{-1}([Z_s] - [Z_c]); \tag{42}$$

Table 2
A comparison of transmission coefficients between theoretical and experimental results for different II-VI semiconductor samples.

Sample	$\|S_{21}\|$(dB)			φ_{21}(°)		
	Test	Ref. [2]	This article	Test	Ref. [2]	This article
CMT78	−3.25	−3.33	−3.32	−63.2	−63.75	−63.01
CMT76	−5.30	−5.19	−5.17	−56.2	−55.77	−56.76
Q154	−8.90	−9.44	−9.44	−28.2	−27.41	−27.20
Q114	−10.65	−10.28	−10.53	31.7	39.22	40.74
Q107	−10.50	−10.47	−10.64	36.8	38.74	39.08
Q105	−10.90	−10.32	−10.51	31.8	38.32	38.20

with

$$[Z_0] = [Q][\overline{Z}_0][Q]_t, \quad (43)$$

$$[Z_s] = [Q][\overline{Z}_s][Q]_t; \quad (44)$$

The matrices $[\bar{Z}_0]$, $[\bar{Z}_s]$ and $[Z_c]$ are all in the diagonal form and their typical elements are given as follows:

$$\overline{Z}_{on} = -j\overline{Z}_n \mathrm{ctg}(\overline{K}_{2n}W/2), \quad (45)$$

$$\overline{Z}_{sn} = j\overline{Z}_n \tan(\overline{K}_{2n}W/2). \quad (46)$$

$$\overline{Z}_n = W\mu/\overline{K}_{2n}, \quad (47)$$

$$Z_{cn} = W\mu/K_{2n}; \quad (48)$$

For the dominant mode, the scattering parameters $S_{21} = S_{12}$ and $S_{11} = S_{22}$ are determined from the first row and the first column of the $[R]$ and $[T]$ matrices, respectively, as:

$$S_{11} = R(1, 1) = \frac{1}{2}[R_0(1,) + R_s(1, 1)], \quad (49)$$

$$S_{21} = T(1, 1) = \frac{1}{2}[R_0(1,) - R_s(1, 1)]. \quad (50)$$

III. NUMERICAL RESULTS

In order to verify the reliability and efficiency of the present method, we calculated the scattering characteristics of different II-VI semiconductor samples. Table 2 presents a comparison of transmission coefficients between the experimental data and the calculated results obtained with the present method and the network method. Very good agreement has been achieved. In our calculation, the number of nodes used is 83, and less than 30 seconds of CPU times are needed for one calculation point on a VAX8700 computer. This demonstrates that the present method has the advantages of accuracy, generality and high efficiency.

REFERENCES

[1] Greiner P. *et al.*, *Digest of 16th Int'l. Conf. on IR and MMW*, 1991, pp. 308-309.
[2] Xu Shanjia *et al.*, *Int. J. Infrared and Millimeter Waves*, 1992; 13(4): pp. 569-587.
[3] Xu Shanjia, *Journal of Electronics*, 1989; 6(3): pp. 232-241.
[4] Xu Shanjia, *Journal of Electronics*, 1989; 6(1): pp. 50-58.
[5] Xu Shanjia *et al.*, *IEEE Trans. Microwave Theory Tech.*, 1989; MTT-37(4): pp. 686-690.