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A. Fenner Milton was born in New York, NY, on October 16, 1940. He received the B.A. degree from Williams College, Williamstown, MA, in 1962, and the M.A. and Ph.D. degrees in applied physics, both from Harvard University, Cambridge, MA, in 1963 and 1968, respectively.

He was a technical staff member of the Science and Technology Division, Institute for Defense Analyses when he joined the staff of the Naval Research Laboratory, Washington, DC, as a Consultant to the Optical Sciences Division. In 1977 he became head of the Electro-Optical Technology Branch. His research interests have included photoconductivity, photo emission, nonlinear optics, integrated optics, and infrared focal plane arrays.

Mode Size and Method for Estimating the Propagation Constant of Single-Mode Ti:LiNbO$_3$ Strip Waveguides

STEVEN K. KOROTKY, WILLIAM J. MINFORD, LAWRENCE L. BUHL, MANUEL D. DIVINO, AND ROD C. ALFERNESS

Abstract—**We have formulated a model to calculate the mode size and propagation constant of single-mode titanium-lithium niobate diffused strip waveguides directly from controllable fabrication parameters and basic constants. The model is compared to measurements of the lateral and vertical mode width of Ti:LiNbO$_3$ waveguides for a variety of diffusion conditions. We show that the model accurately predicts the geometrical mean mode size of the two-dimensional waveguide. The model provides a simplified method for estimating the mode size and propagation constant of the guide, and is useful in designing waveguide devices having low fiber/waveguide coupling and bending losses.**

I. Introduction

Optical waveguides produced by the in-diffusion of titanium into lithium niobate crystals have been used to fabricate many electrooptic and acoustooptic devices which are potentially useful for communication and sensing application [1]. The successful construction of some of these devices, directional coupler wavelengths filters [2], for example, depends critically on engineering the propagation constants of the waveguides. For other applications, such as coupling to a fiber [3], it is also necessary to control the size of the waveguide mode. For the most part, research devices based on Ti:LiNbO$_3$ waveguides are developed through trial and error iteration. As devices continue to become increasingly more complex, the need for simple physical models for estimating and relating the mode parameters of Ti:LiNbO$_3$ single-mode strip waveguides becomes more acute.

In this paper, we present measured mode sizes for Ti:LiNbO$_3$ waveguides as a function of several diffusion parameters. We also describe a model, based on the variational principle for the propagation constant, which predicts the characteristics of single-mode diffused strip waveguides in terms of controllable diffusion parameters. The model accurately reproduces the experimental geometrical mean mode size from fundamental parameters, and also provides a simplified method for estimating the propagation constant of diffused strip waveguides.

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S. K. Korotky, L. L. Buhl, M. D. Divino, and R. C. Alferness are with Bell Laboratories, Holmdel, NJ 07733.
W. J. Minford is with Bell Laboratories, Allentown, PA 18103.

II. Experiment

A. Waveguide Fabrication

The waveguides used in the experiments were fabricated on z-cut, y-propagating LiNbO$_3$ crystals having an acoustic grade polish. Waveguide patterns were produced using standard photolithographic techniques. On one crystal, a set of 720 Å thick Ti strips ranging in width from $1\frac{1}{2}$ to 10 μm in $\frac{1}{2}$ μm steps was evaporated. The metal was in-diffused for 6 h at 1100°C. On three other crystals, 6 μm wide Ti strips were prepared with thicknesses of 740, 850, and 1110 Å. The diffusion condition for these crystals was 1050°C for 6 h. In all cases, the diffusion was carried out in an H_2O rich atmosphere to prevent surface guiding due to Li out-diffusion. The ends of the waveguides were blocked and optically polished to achieve flat end surfaces.

B. Mode Profile Measurements

Waveguide mode sizes (full width at half maximum power intensity Γ) in the directions parallel to and perpendicular to the crystal surface were measured for both TE and TM polarizations at the 1.32 μm wavelength using an Nd-YAG laser.

One-dimensional cuts of the 2D-mode profile, which intersect the peak power point, were obtained using a technique similar to that used by Chen and Wang [4] to study mode confinement in semiconductor lasers. The near-field pattern was

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imaged onto an IR-sensitive camera placed approximately 1.5 m from the end of the waveguide. A magnification of approximately 375X was obtained by using a 4 mm focal length/0.65 NA microscope objective located near the LiNbO$_3$ crystal. The absolute magnification of the system was determined to an accuracy of about 5 percent by magnifying the two outputs of an integrated directional coupler with calibrated center to center waveguide separation at the ouput ports. The imaging resolution set by diffraction from the lens aperture stop is approximately 1 μm.

The video signal from the camera tube was simultaneously displayed on a TV monitor and the CRT of a digital storage oscilloscope; this combination facilitated critical focusing. Measurements of the mode shape were recorded using the oscilloscope. The digital feature significantly enhanced the measurement accuracy since it permitted signal averaging to reduce random tube noise to a negligible level, allowed subtraction of the black-level background—which is often not constant across a TV scan line—to avoid systematic offset errors, and eliminated the need to make measurements directly from the CRT screen.

C. Experimental Results

The experimental values for the full width at half maximum intensity parallel to (lateral) and perpendicular to (vertical) the crystal surface and for the various diffusion parameters are summarized in Figs. 1 and 2. The data are for the TM polarization. The results for the TE mode are very similar except the mode sizes are slightly larger, which is a result of the smaller index difference produced for the same Ti concentration. In the single-mode region examined, the mode sizes generally decrease with increasing initial metal strip width W and metal thickness τ, when all other variables are held constant, as a result of stronger optical confinement. If the strip width is increased further, and the multimode region is approached, the size of the fundamental mode is expected to pass through a minimum.

It is not possible to compare the relative mode confinement or relative effective index for the waveguides of Fig. 1 to those of Fig. 2, based solely on the experimental mode sizes, because the parameters of the index distributions are quite different for the two. In general, the propagation constant is determined by the difference between two competing terms. One term depends inversely on the square of the mode size. The other term depends on the overlap of the field distribution with the index distribution. This is made clear below, where we present a model for the waveguide parameters based on the variational principle for the propagation constant. The model predicts the mode sizes from fundamental parameters and in turn relates the mode sizes to the effective index.

III. Model

A. Theory

Approximations for the propagation constant of dielectric waveguides having arbitrary index distributions can be obtained using variational principles [5]-[7]. We apply the variational method here to calculate the mode characteristics for single-mode diffused strip waveguides.

The index difference used to produce single-mode waveguides via metal in-diffusion is small. Marcatili [8] has shown that, when the index of the guiding region of rectangular-type waveguides differs only slightly from the bulk index, the supported modes are essentially TEM in nature. We assume, therefore, that the major field components of the modes are perpendicular to the direction of propagation, and are polarized either perpendicular to (TM) or parallel to (TE) the crystal surface. Because the index difference is small, the field components satisfy the scalar wave equation [9]

$$\nabla^2 \vec{E} = \mu_0 \epsilon \frac{\partial^2}{\partial t^2} \vec{E}$$

where μ_0 is the free space permeability and ϵ describes the

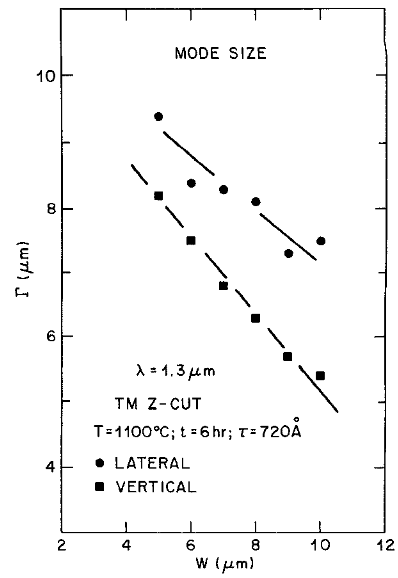

Fig. 1. Experimental Ti:LiNbO$_3$ mode sizes I. The figure shows the measured full width at half maximum intensity (Γ) in width (lateral) and in depth (vertical) as a function of the initial metal strip width (W) of the single-mode waveguide. The data are for fixed diffusion temperature (T) and time (t) and for fixed metal thickness (τ). Lines passing through the data are merely to guide the eye.

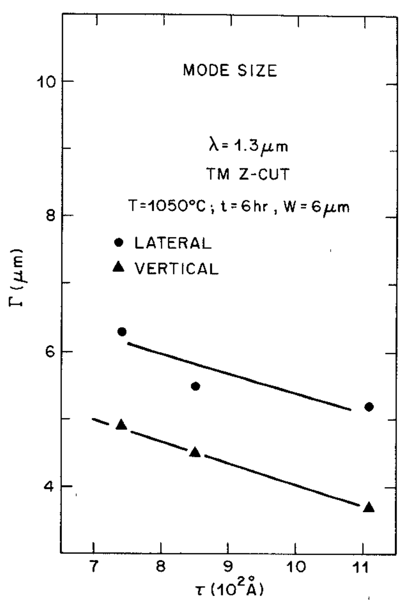

Fig. 2. Experimental Ti:LiNbO$_3$ mode sizes II. Measured mode sizes in the lateral and vertical directions are plotted as a function of metal thickness for fixed metal strip width. The diffusion temperature and time are also constant, but differ from the value in Fig. 1. Again, the lines passing through the data are merely to guide the eye.

permittivity of the structure. To be explicit, we consider the propagation of a monochromatic wave of frequency ω traveling along the y-axis and polarized parallel to the z-axis. The wave equation for $E_z(x,z)$ is

$$\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial z^2}\right)E_z(x,z)+n^2(x,z)\,k^2E_z(x,z)=\beta^2E_z(x,z)$$

where β is the propagation constant, and we have defined, as is customary,

$$\epsilon_0 n^2(x,z)=\epsilon(x,z),$$

and $k^2=\mu_0\epsilon_0\omega^2$, with ϵ_0 the free space permittivity.

Since the index distribution $n(x,z)$ differs only slightly from the bulk index, we write $n(x,z)=n_B+\Delta n(x,z)$. To an acceptable approximation, the index change produced by diffusion is directly proportional to the metal concentration density for polarization along the extraordinary axis of $LiNbO_3$ [10]. Also, if the diffusion is isotropic, the metal concentration density is separable [11]. Thus, we may write

$$\Delta n(x,z)=\Delta n_0 f(x)\,g(z)$$

where f and g are the concentration profiles and Δn_0 is a constant.

When the diffusion time is long compared to the time required to exhaust the source of metal, which is usually the case, the function describing the diffusion distributions are [11]

$$f(x)=\left\{\operatorname{erf}\left[\frac{1}{\sqrt{2}D}\left(x+\frac{W}{2}\right)\right]-\operatorname{erf}\left[\frac{1}{\sqrt{2}D}\left(x-\frac{W}{2}\right)\right]\right\}\Big/2\operatorname{erf}\left(\frac{W}{2\sqrt{2}D}\right)$$

and

$$g(z)=\exp-\frac{1}{2}\left(\frac{z}{D}\right)^2.$$

Here W is the initial metal strip width and D is a diffusion depth. The diffusion depth is expressed as $D=(2\mathfrak{D}t)^{1/2}$ where $\mathfrak{D}$ is the diffusion constant and t is the diffusion time. The temperature (T) dependence of $\mathfrak{D}$ is given by $\mathfrak{D}=\mathfrak{D}_0e^{-T_0/T}$ where T_0 is a constant.

The constant Δn_0, which represents the peak index change, is determined by requiring that the number of metal atoms before and after diffusion be identical. Enforcing the conservation of atoms, one finds $\Delta n_0=(dn/dc)\cdot\operatorname{erf}(W/2\sqrt{2}D)\cdot\sqrt{2/\pi}\,(\tau/D)$, where dn/dc is the change in index per unit change in metal concentration. This expression is true for polarization along the extraordinary. For polarization along the ordinary crystal axis, Δn is not directly proportional to the metal concentration, and so the formalism developed is not strictly valid. However, the direct relationship may be used as an approximation if (dn/dc) is interpreted as an effective constant. A value for (dn/dc) representative of the region of the peak concentration $\operatorname{erf}[W/2\sqrt{2}D]\sqrt{2/\pi}\,(\tau/D)$ will serve as an estimate in this case.

To apply the variational principle, an ansatz for the mode profile is required. Taylor [7] has applied the variational method to diffused waveguides by expanding the mode profiles as a sum of products of parabolic cylinder functions and retaining 21 terms. This large number precludes a direct physical correspondence between individual mode size parameters and measurable spot sizes unless a single term dominates the series. At present, however, we are interested only in the properties of the fundamental mode. It has been found experimentally [12] that the shape of the fundamental mode of diffused strip waveguides is to a good approximation Gaussian in width and Hermite-Gaussian in depth. Therefore, as a simplified form for the functional dependence of $E_z(x,z)$, we consider a product solution $E_z(x,z)=\psi(x)\,\phi(z)$ with normalized profiles:

$$\psi_w(x)=\frac{1}{\sqrt{(w/2)\sqrt{\pi}}}\exp-\frac{1}{2}\left(\frac{x}{w/2}\right)^2$$

and

$$\phi_d(z)=\frac{2}{\sqrt{d\sqrt{\pi}}}\left(\frac{z}{d}\right)\exp-\frac{1}{2}\left(\frac{z}{d}\right)^2$$

where d and w are the mode size parameters for depth and width.

Because the index distribution does not differ greatly from n_B, the propagation constant will not vary substantially from n_Bk. Introducing the effective index N with $\beta=Nk$, we write $\beta=(n_B+\Delta N)\,k$. The variational equation for the effective index difference ΔN is then

$$2n_B\Delta Nk^2=\int dx\,\psi(x)\,\frac{d^2\psi(x)}{dx^2}+\int dz\,\phi(z)\,\frac{d^2\phi(z)}{dz^2}+2n_B\Delta n_0k^2\int dx\,\psi^2(x)f(x)\cdot\int dz\,\phi^2(z)\,g(z)$$

which is obtained from the wave equation by left multiplying by $(\psi\phi)^*$ and integrating over the x–z surface. We have also made use of the hypothesis that $n(x,z)\simeq n_B$.

When the trial solution is substituted into the above equation, and the integrations are carried out, we derive the following relationship among ΔN, d, and w:

$$\begin{aligned}2n_B\Delta NW^2k^2&=\frac{-9}{2(D/W)^2\,(d/D)^2}-\frac{4}{2(w/W)^2}\\&\quad+\left(2n_B\left(\frac{dn}{dc}\right)\tau Wk^2\right)\left(\frac{W}{D}\right)\\&\quad\times\sqrt{\frac{2}{\pi}}\left(1+\frac{1}{2}\left(\frac{d}{D}\right)^2\right)^{-3/2}\\&\quad\times\operatorname{erf}\left(1/\sqrt{(w/W)^2+8(D/W)^2}\right)\\&\equiv F(d,w).\end{aligned}$$

We now apply the variational principle by making use of the fact that the propagation constant is stationary with respect to variations in the eigenfunction solution; the true solution ΔN_s always satisfies $2n_B\Delta N_sW^2k^2\geqslant F(d,w)$. Thus, the parameters d and w are determined by maximizing $F(d,w)$ for given diffusion conditions. In so doing, this model differs from the effective index method [11], [13], [14] in that the contributions to confinement from the orthogonal spatial directions are handled simultaneously in the present case. Also, it is evident from the previous equation that the effective index difference is determined by the competition between two types of terms. One type depends on the overlap of the *normalized* mode distribution with the index distribution and is maximized for smaller mode sizes. The other type decreases as the inverse of the square of the mode sizes and prevents the mode from collapsing. Finally, we emphasize that the ultimate accuracy of the values obtained for d and w depends on how closely the form of the trial wave function resembles the true solution.

B. Calculations

We have calculated normalized mode sizes and normalized dispersion curves for the fundamental mode of diffused strip waveguides using the model outlined above. The present model has the advantage that the maximization of F can be reduced to a one-dimensional problem by using either one of the required relations: $\partial F/\partial w = 0$ or $\partial F/\partial d = 0$. Using this simplification, the maximization procedure was carried out numerically. Fig. 3 shows the calculated normalized mode sizes as a function of the dimensionless strength parameter $2n_B(dn/dc)\ \tau W k^2$ for various values of the D/W ratio. The *normalized* mode sizes decrease with the increasing value of the strength parameter, and approach a constant for large τ or W. In Fig. 4, we graph the corresponding normalized dispersion relations.

To compare the model with the experiment, we have used it to calculate the expected mode sizes for the diffusion conditions corresponding to the experiment. The value of $(dn/dc)_e = 0.625$ (concentration in fraction of that of pure Ti metal) for the extraordinary axis was taken from the work of Minakata *et al.* [10]. The temperature coefficient T_0 has been measured by Naitoh *et al.* [15], and is approximately 3.03×10^4 K. Uncertainty in the value of $\mathfrak{D}_0$ is somewhat larger than those of the other fundamental parameters. We have found that a value of $\mathfrak{D}_0 = 2.3 \times 10^{-2}$ cm^2/s provides a good description of the present waveguides. This value is close to the value of 1.4×10^{-2} cm^2/s, which can be extracted from the data for strip waveguides of Fukuma *et al.* [16]. It is important to note that with the above assignment of constants, there are *no* free parameters in the model.

In Fig. 5, we compare the model calculations, for the values of the fundamental parameters stated above, to experiment by considering the geometrical *mean* size of the mode, i.e., $\sqrt{\Gamma_d \Gamma_w}$. Note that the full widths at half maximum intensity $\Gamma_{w,d}$ are related to the model field parameters (w, d) by $\Gamma_w \simeq 0.83w$ and $\Gamma_d \simeq 1.16d$. Considering the simplifying assumptions of the model, and that the diffusion depth for the higher temperature is greater than 1.5 times larger than that of the lower temperature, the agreement with the experiment is remarkably good. The model does not do as well when trying to reproduce the *ratio* of the mode sizes Γ_d/Γ_w, as is seen in Fig. 6. Calculated values are systematically larger by about 20 percent. This discrepancy may be attributable to the fact that the model values represent an average over the entire two-

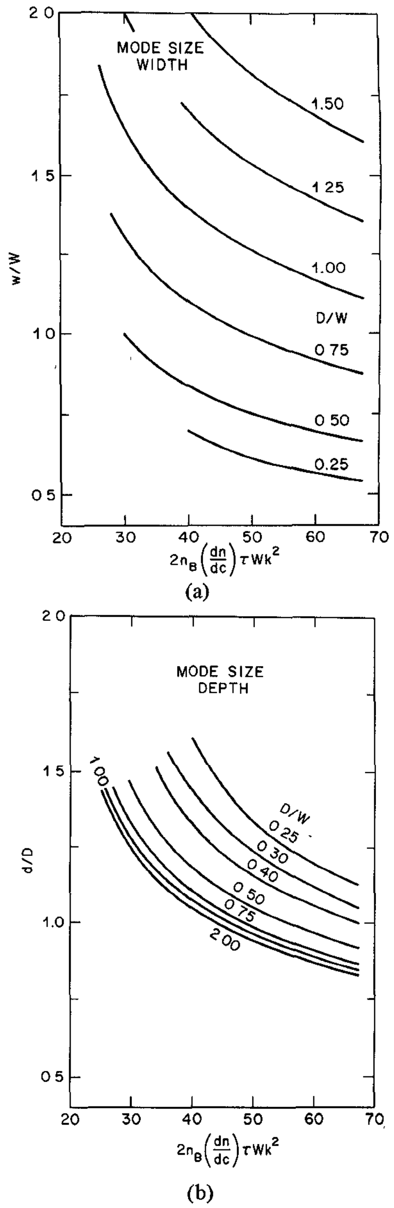

Fig. 3. Normalized mode sizes. Calculated mode sizes in (a) width w/W and (b) depth d/D are plotted as a function of the dimensionless strength parameter $2n_B(dn/dc)\ \tau W k^2$. This combination of variables occurs naturally in the model (see text). The calculations were carried out for several values of the diffusion depth (D) to strip width (W) ratio.

dimensional mode profile, whereas the experimental widths were measured only for the peak power point. It is possible that the actual mode size aspect ratio, when averaged over the entire two-dimensional profile, is closer to unity than the present measurements indicate. Alternatively, the observed mode asymmetry may be a result of anisotropy in the diffusion process, which is not incorporated in the present model. Measurements of the full 2-D mode profiles are required to investigate these possibilities.

Values for the effective index difference calculated for the experimental diffusion conditions are plotted in Fig. 7 to illustrate the potential usefulness of the model in estimating ΔN. The model indicates, for example, that the effective index difference for the smaller diffusion depth is increased by roughly 0.9×10^{-3} for each 200 Å increment in τ above the initial

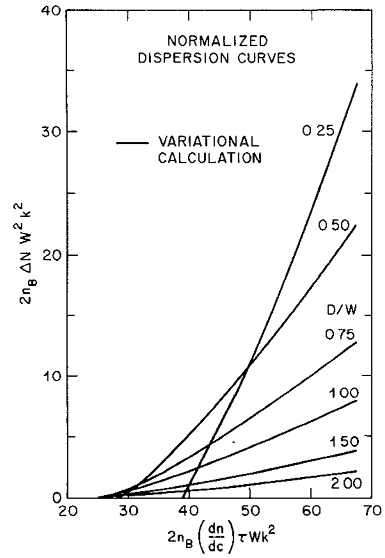

Fig. 4. Normalized dispersion curves. Dispersion curves for the fundamental mode of diffused waveguides obtained using the variational principle are graphed for several values of the D/W ratio.

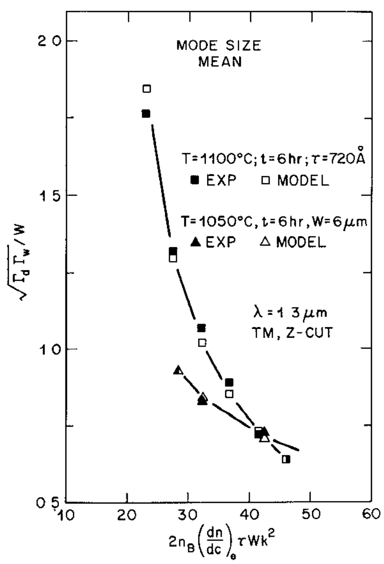

Fig. 5. Geometrical mean mode size. Model calculations for the geometrical mean mode size $\sqrt{\Gamma_d \Gamma_w}$ are compared to the experimental data of Figs. 1 and 2. The comparisons are made on the same graph by using the dimensionless model variable $2n_B(dn/dc)\ \tau W k^2$, which is directly proportional to the product τW, for the abscissa. The diffusion depth for the larger temperature is approximately 1.5 times greater than the diffusion depth for the lower temperature.

metal thickness of approximately 700 Å required to establish reasonable mode confinement. This is consistent with an independent analysis of recent bending loss measurements for these waveguides [17].

IV. Summary

We have made measurements of the mode sizes for single-mode Ti:$LiNbO_3$ strip waveguides for a variety of diffusion conditions. A model for the mode characteristics of these waveguides has been formulated using the variational principle for the propagation constant. The model relates the mode size

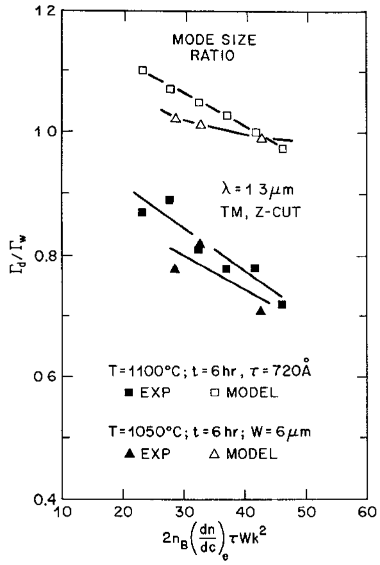

Fig. 6. Mode size ratio. Model calculations for the mode size aspect ratio Γ_d/Γ_w are compared to the experimental data. The model systematically overpredicts the measured ratio by approximately 20 percent. This suggests that the mode size aspect ratio, when averaged over the entire two-dimensional profile, may be closer to unity than the experimental data indicate.

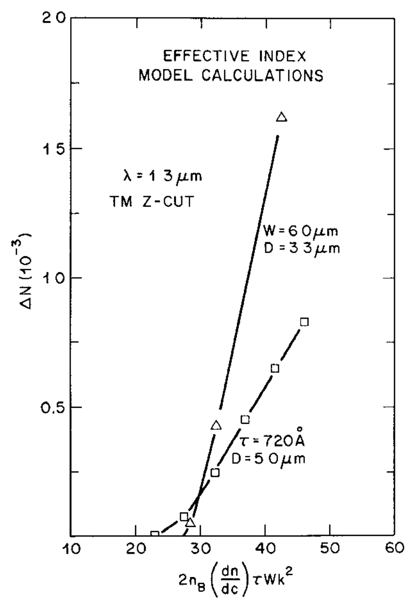

Fig. 7. Effective index difference. The figure shows model calculations of the effective index difference for the diffusion conditions corresponding to the experimental mode size data (see Fig. 5). The values for fixed strip width (Δ) are consistent with bending loss measurements for identical diffusion conditions. Note that the effective index difference for the diffusion condition T = 1050°C, t = 6 h, τ = 1110 Å, and W = 6 μm is calculated to be almost twice as large as for T = 1100°C, t = 6 h, τ = 720 Å, and W = 10 μm.

to the effective index of the guide and to controllable diffusion parameters. We have found that the model can accurately reproduce the experimental values for the geometrical mean of the mode sizes using values for basic constants consistent with the literature. The model is potentially useful in designing waveguide devices.

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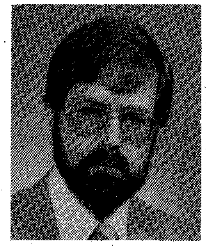
Steven K. Korotky was born in Paterson, NJ, on February 13, 1953. He received the B.A. degree in physics from Rutgers University, New Brunswick, NJ, in 1975, and the M.S. and Ph.D. degrees in physics from Yale University, New Haven, CT, in 1976 and 1980, respectively. His thesis work was on nuclear molecular states formed in heavy-ion collisons.

He joined Bell Laboratories, Holmdel, NJ, in August 1980, and is currently working on optical guided wave devices.

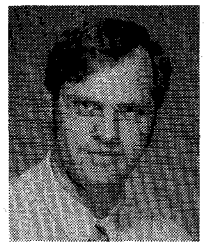
Dr. Korotky is a member of the American Physical Society.



William J. Minford was born in Bethlehem, PA, on September 25, 1949. He received the B.S., M.S., and Ph.D. degrees in ceramic science from the Pennsylvania State University, University Park, in 1971, 1973, and 1977, respectively.

He joined Bell Laboratories, Allentown, PA, in 1976 where he is currently working on guided wave optical devices.

Dr. Minford is a member of the American Ceramic Society and Sigma Xi.



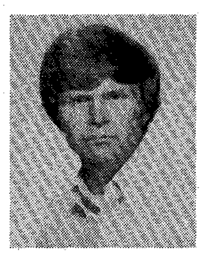
Lawrence L. Buhl was born in Norfolk, VA, on November 6, 1948. He attended A.T.E.S. Technical School, Erie, PA, from 1966 to 1968 where he studied electronic engineering technology.

At present, he is completing work on the B.S. degree in electronic engineering at Monmouth College, Long Branch, NJ. From 1968 to 1971 he was a member of the U.S. Army Signal Corps, Fort Monmouth, NJ, where he taught microwave theory and radar systems repair. He joined Bell Laboratories, Holmdel, NJ, in 1972, and is currently working on guided wave optical devices.

Mr. Buhl is a member of Eta Kappa Nu.

Manuel D. Divino was born in Manila, Philippines, on September 5, 1935. He received the B.S. degree in agricultural engineering from the University of the Philippines, Los Banos, in 1957, the A.A.S. degree in electronics engineering technology from the RCA Institute, New York, NY, in 1967, and the B.S. degree in electrical engineering from Newark College of Engineering, Newark, NJ, in 1975.

He has worked at Bell Laboratories, Holmdel, NJ, since 1967 in the area of gas lenses, optical fibers, and integrated optical devices.



Rod C. Alferness received the B.S. degree in physics from Hamline University, St. Paul, MN, in 1968, and the M.S. and Ph.D. degrees in physics from the University of Michigan, Ann Arbor, in 1970 and 1976, respectively. His thesis work was on optical diffraction in thick holographic gratings.

From 1970 to 1972 he was a member of the U.S. Army, Fort Monmouth, NJ, where he performed theoretical studies of laser propagation in the atmosphere. He joined Bell Laboratories, Holmdel, NJ, in June 1976, where he has been engaged in research on optical guided wave devices, including switches, modulators, wavelength filters, and polarization controllers.