SIMULATION AND DESIGN OF AN ORGANIC QUANTUM FILM ELECTROOPTIC SWITCH

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Abstract In this paper the simulation and design of a quantum-film electrooptic switch is considered. This photonic device, is made from a new organic dipolar material called MNA or 2-methyl-4 nitroaniline, which possesses a high merit in comparison with it's inorganic counterparts (e.g. $LiNbO_3$, GaAs, InSb, Quartz, etc). MONTECARLO method is used to simulate the photon-π-electron interaction in this material and the introduced physical model is based on wave-particle nature of light to demostrate the POCKELS' Electrooptic effect in MNA optical switch. The main advantages of this design are wide optical bandwidth (0.5 -2 microns wavelegnth), low power consumption and high speed data transmission.

Key Words Quantum-Film, Electrooptic Effect, Pockels, Benzene Family, Montecarlo Method, Optical Switch, Ordinary and Extraordinary Refractive Indices, Phase Retardation, First Quarter Wave Thickness

چکیده در این مقاله به چگونگی شبیه سازی و طراحی یک سوئیچ نوری در ابعاد کوچک (میکرومتر) پرداخته شده است. این سوئیچ از جنس یک ترکیب کریستالی آلی از خانواده بنزن موسموم به «۲ ـ متیل ـ ۴ نیتروآنیلین» (ام ـ ان ـ آ)، می باشد. ماده کریستالی فوق در مقایسه با مواد معدنی اپتیکی همچون لیتیوم نیوباید، کوارتز، گالیم ارسنایید و غیره، از نظر فعالیت نوری، به مراتب قویتر است. ضمن این تحقیق، ما با استفاده از روش شبیه سازی مونت کارلو، به تشریح نحوه واکنش نور برخوردی با الکترونهای «پی» حلقه های بنزنی در کریستال مزبور می پردازیم. مدل فیزیکی بکار گرفته ضمن این شبیه سازی ، طبیعت موج ذره ای فتون را حین واکنش با ماده در مد نظر قرار می دهد و بدین ترتیب ما توانسته ایم اثر مهم الکترواپتیک را که عامل اصلی ایجاد سوئیچینگ نوری در این ماده است شبیه سازی نمائیم. از مزیات مهم طرح این سوئیچ، پهنای باند نوری زیاد (از طول موج ۰/۵ تا ۲ میکرون)، مصرف توان کم و انتقال سریع اطلاعات می باشد.

INTRODUCTION

The rapid development of organic optical materials is due to their electronics delocalization and large electron-electron interaction. They have the potential for fast swithching, large capacity information processing and high density date transmission which are the needs of optical communication systems.

The main features of binary optical communication links are the source of light (laser), the optical switchs, fibers and optical receivers. For realizing optical communication, inorganic crystals have been the best candidate till now and (III-V) & (II-VI) groups of materials have already been widely used for realization of semiconductor lasers, optical modulators, switchs, amplifiers and photodetectors. [1,2] Also, inorganic electrooptic materials like $LiNbO_3$, have been the main material candidates for optical modulation and nonlinear optical phenomena as Harmonic generation, parametric oscillation, etc. [3,4,5,6].

In this paper a new noncentrosymmetric organic compound is introduced which has shown some merits necessary for realization of optically controlled devices.

A design procedure is suggested for quantum film

optical switch made from an aromatic material called: 'MNA". Because of it's microscopic dimensions, it is suitable for optical integrated or hybrid circuit realization. This organic electrooptic switch can provide three main advantages in optical communication at the same time. First is wide optical bandwidth. Experimental measurements at Bell Laboratories [7] have shown that MNA is transparent in a wide optical spectral region- from 0.5 micron wavelength in visible band to 2 microns in far infrared region. Therefore, one can use different single-mode lasers at very different optical wavelengths [λ_1, λ_2, ... λ_m], to be switched by electrical signals. By using photodetectors with narrow band frequency responses at λ_1 or λ_2 .. or λ_m, it'll be possible to send a specific message to specific receiver channels (Figure 1). Seconds is low power consumption. "MNA" is an insulator and does not load the external voltage source (Vs)-(see Figure1). Third is high bit rate data transmission. Because of it's small dimensions in length (L<200 microns), width (W < 10 microns) and depth (d < 1 microns), capacitance of the device will be in the range of 10^{-13} farad or less, so that the switching speed will be in the range of 100 gigabits per second.

To analyse such a quantum film switch, the classical methods can no more be used [2, 13, 17, 26]. As concepts such as refractive index, refraction angle and phase retardation lose validity in shrinking devices, more rigorous approaches are becoming necessary. The most direct approach is to simulate the microscopic electron - photon interaction. By averaging the results, one can obtain the average index of refraction, or phase retardation in a specific material.

In our previous works, first of all we've introduced a generalized model for MESFET photodetectors suitable for optical detection of signals received

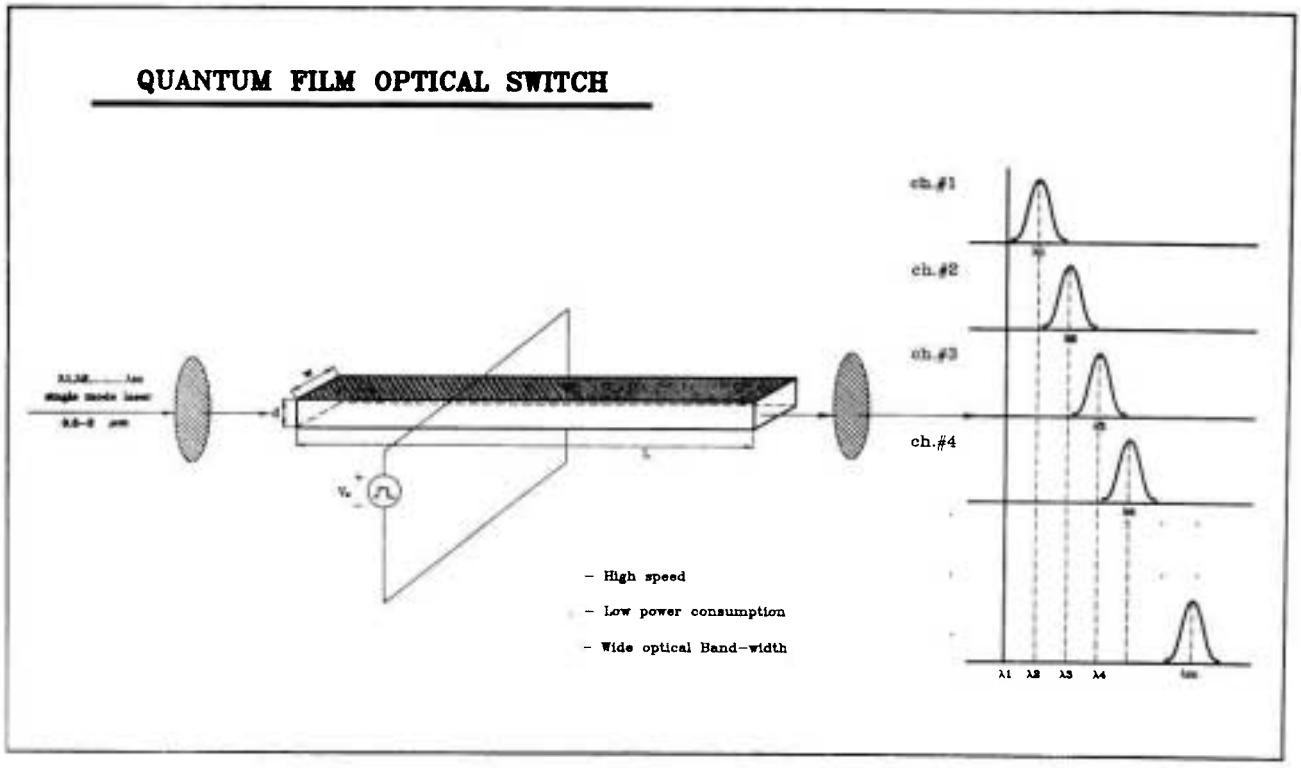


Figure 1. A quantum film Electro-optic switch made of an organic material called MNA. The main advantages of this switch are wide optical bandwidth, lowpower consumption, high speed data transmission.

from a wideband optical modulator [1]. Then we searched for a candidate material suitable for wideband optical modulator and analysed it in detail [7, 9, 10, 11, 12]. We selected an aromatic hydrocarbon (MNA) from the Benzene family and introduced a physical model based on wave-particle nature of light to estimate theoretically the fluctuations of refractive indices and also phase retardation at submicron scales [13, 14]. "MNA", possesses important linear and nonlinear optical properties for realizing optically controlled devices, comparing with their inorganic counterparts.

In this paper we have suggested a practical design to make a wide-band electrooptic switch, from MNA and we will analyse the Pockels electrooptic effect in this material.

In Section I, we'll describe in brief the molecular structure of MNA in Benzene group. In Section II, we'll explain the classical methods for analysing the wave-matter interaction, and why it is not applicable to the so called quantum film modulator. Our proposed physical model to predict electrooptic effect in this modulator will be introduced at Sections III and IV.

In the concluding section, we'll compare the results of our research with the expermental measurements obtained previously. [7, 12].

I. "MNA, AN AROMATIC HYDROCARBON"

"MNA", or 2-methyl-4-nitroaniline, is a member of Benzene group where methyl (CH_3), amino (NH_2) and nitro (NO_2) are substituted for three hydrogen atoms. Single-crystal X-ray diffraction studies of MNA, determined the space group to be monoclinic, with four molecules per unit cell (see Figures 2,3) [7,9,12].

Some of the electrons associated with the carbonic double bonds are not actually localized between specific atomic pairs, but revolve around the entire ring. These electrons, known as π-Electrons, are thus delocalized are their wavefunctions are of particular interest in this paper.

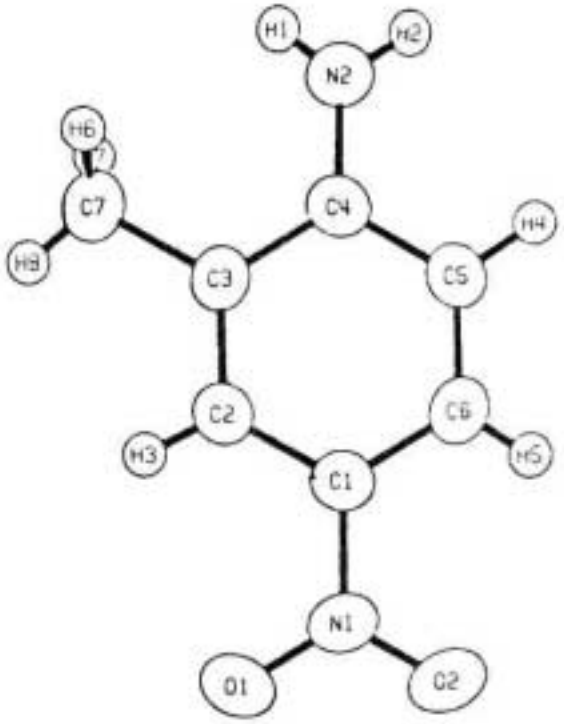


Figure 2. The Molecular Structure of 2-Methyl-4-Nitroaniline (MNA), as determined by X-ray crystallography. Key: C, carbon; N, nitrogen; O, oxigen; and H, hydrogen. MNA Monoclinic Crystal.

To obtain π-Electron wavefunction ψ, the Schrödinger equation may be solved. Since this can not be done exactly, an approximated procedure known as Huckle method must be employed. In this method using Tight-binding model, Molecular Orbital (MO) is taken to be a linear combination of atomic orbitals. That is:

$$\psi = \Sigma_r C_r \phi_r \qquad (1)$$

Where the ϕ_r refers to atomic orbitals of carbon atoms in the ring, and the summation is over the six C atoms. The C_r's are constants to be determined. The Schrödinger equation for a delocalized electron is:

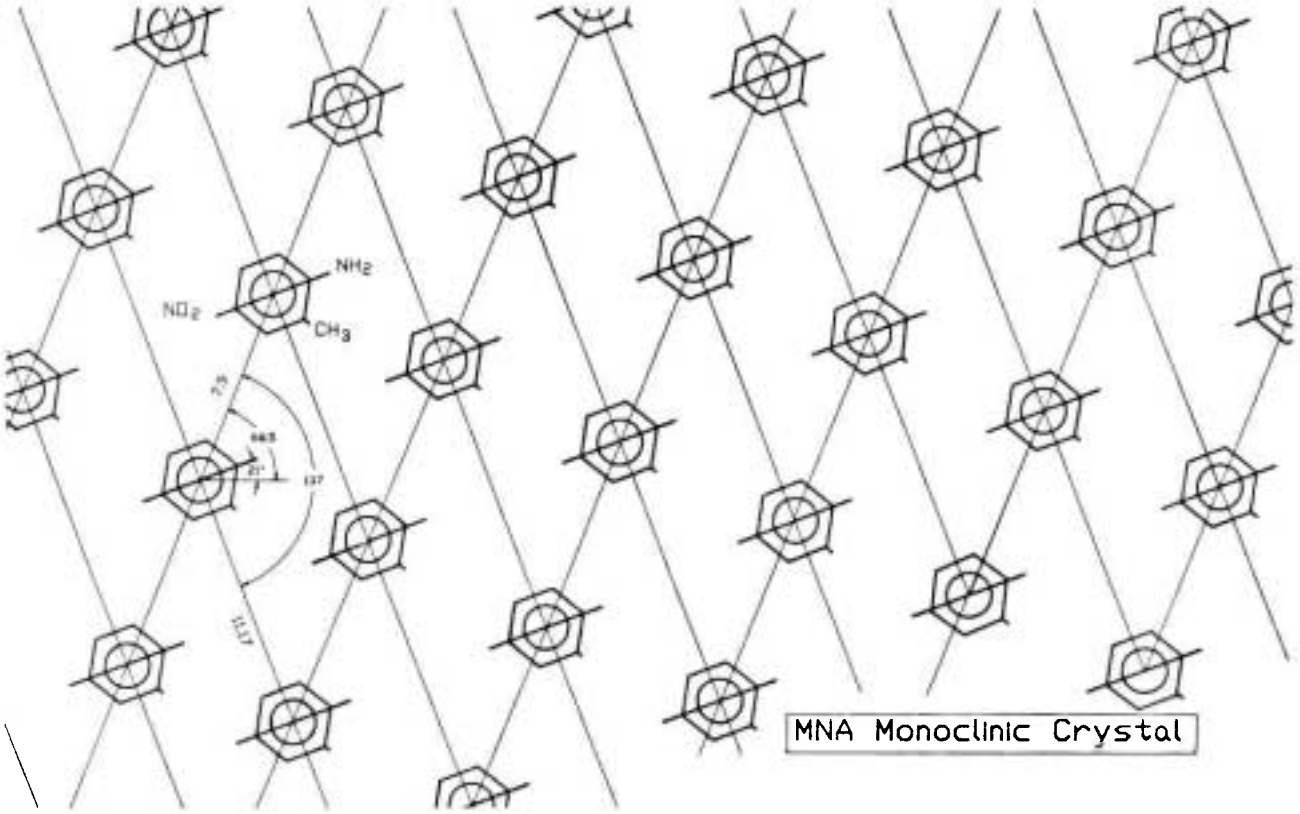


Figure 3. Single-Crystal X-ray diffraction studies of MNA, determined the space group to be Monoclinic, with four molecules per unit cell.

$$[-\frac{h^2}{2m}\nabla^2 \Sigma_r V_r]\,\psi = E\psi \qquad (2)$$

Where V_r is the atomic potential of r'th atom. Following the common approach in quantum mechanics, we multiply the above equation from the left by, ϕ_1, ϕ_2, ϕ_3, ... , respectively, and integrate over space in each case. Solving this set of algebraic equations, The C'$_r$th coefficient, the wavefunction and energy E will be determined. Thus $|C_1|^2$ is the probability of the π-electron at atom no.1, $|C_2|^2$ the same for atom no.2, and so forth. Thus,

$$|C_1|^2 + |C_2|^2 + \ldots + |C_6|^2 = 1 \qquad (3)$$

In the case of Benzene, $|C_r|^2 = 1/6$, as follows from the symmetry of the ring [6, 15]. But in MNA, where there is no symmetry, the probability of finding the π-electrons at various atoms will be different. We'll discuss in section III a proposed position probability of π-electrons for MNA. MNA is a double - refractive material which causes phase retardation between ordinary and extraordinary components of incident light travelling inside the crystal. We'll explain this phenomenon in the following section.

II. CLASSICAL METHOD

An understanding of wave propagation in transparent anisotropic crystals is prerequistite to the treatment of a number of important phenomena as refraction, phase retardation, electroopic and magnetooptic effects and also nonlinear phase - matching condition regarding the Second Harmonic Generation (S.H.G.) in noncentrosymmetric crystals.

In classical approach to these phenomena, the MAXWELLS' equations help us analyse the macroscopic behavior of electric and magnetic fields of incidents light (E&H), travelling inside the crystal [3, 20]:

$$\nabla \times H = i + \frac{\delta D}{\delta t}$$
$$\nabla \times E = -\frac{\delta B}{\delta t} \qquad (4)$$

Where "i" is the current density, and the consitutive equations relating the polarizations of medium (P & M) to the displacement vector (D & B) are: [4]

$$D = \varepsilon_0 E + P$$
$$B = \mu_0 (H + M) \qquad (5)$$

In anisotropic crystals, the above equations are direction dependent so they are in Matrix forms and the constitutive parameters are tensors. For instance the electric displacement vector D and the electric field E in uniaxial crystals are related by means of dielectric tensor: [4,5]

$$\frac{1}{\epsilon_0} \times \begin{bmatrix} D_x \\ D_y \\ D_z \end{bmatrix} = \begin{bmatrix} 1+\chi_p & 0 & 0 \\ 0 & 1+\chi_s & 0 \\ 0 & 0 & 1+\chi_s \end{bmatrix} \begin{bmatrix} E_x \\ E_y \\ E_z \end{bmatrix} \qquad (6)$$

So that we can define the microscopic Ordinary (no) and extraordinary (ne) indices of refractions as follows:

$$no = (1 + \chi_s)$$
$$ne = (1 + \chi_p) \qquad (7)$$

It means that if incident light at different polarization angles travels inside these kinds of crystals, it causes two perpendicular components (ordinary & extraordinary) which will have different velocities leading to phase retardation [3, 22].

$$\Delta\phi = \frac{(no - ne).L.W}{C_0} \qquad (8)$$

Also the variation of refractive index due to external electric field in noncentrosymmetric crystal lattices are responsible for linear electrooptic pockels effect. The phase retardation, (Γ), with an applied electric field in a typical linear transverse electroopic modulator will be obtained as follows: [4, 5, 7]

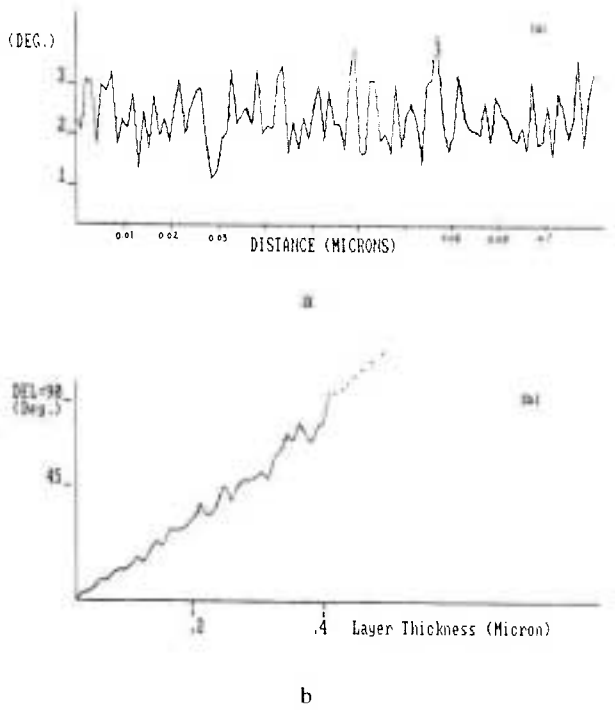
$$\Gamma = \frac{\omega}{C}\left[(n_0 - n_e) - \frac{n_0^3}{2} r63 \left(\frac{V}{d}\right)\right] \qquad (9)$$

Where d is the crystal thickness, no & ne, the ordinary and extraordinary indices of refractions at optical frequency ω, and v is the applied voltage.

In Equations 4 to 9 the assumption of constant macroscopic constitutive parameters (no & ne) are derived trom averaging microscopic fluctuations of parameters as the material's thickness becomes enough large.

But these parameters lose their validities as device dimensions shrink to submicrometers. In submicron dimensions the refractive indices will no more be constant but rather fluctuate around mean values [13, 16]. The problem is solved in molecular scale using MONTECARLO method for photon - electron interaction. MONTECALRLO method has already been used for electron - lattice interaction in solid state devices [17, 18, 19] to obtain average carrirer density, velocity, energy and other quantities of interest as a function of position, within the semiconductor devices.

In our previous works [13, 14], we have introduced a physical model based on wave - particle nature of light to estimate theoretically the fluctuations of refractive indices and also phase retardation



b

Figure 4. a) Spatial phase retardation fluctuations in every 100 Angstroms thickness of MNA monoclinic crystal. **b)** First Quarter Wave thickness for MNA at wavelength: 6328 A and ellipse eccentricity = 0.8 (Simulated by Montecarlo method.

at submicron scales. (Figure 4 & Table I). The candidate material for simulation was MNA. In this paper we've also simulated the pockels effect in this organic material.

III. THE PHYSICAL MODEL

The speed of light in vacuum is c = 300000 km/sec. But when travelling inside a transparent dense material, it'll be reduced by a factor of n. "no" & "ne" are macroscopic quantities called index of refraction describing the wave-matter interaction and explaining photon travelling delay. In double refractive materials "n" depends on polarization direction of incident light.

Let's assume a microsscopic delay, τo_i, for i'th. molecule of matter when interacting with photon travelling in ordinary direction and another delay,

TABLE I. First Quarter Wave (FQW) thickness (Ellipse's eccentricity = 0.8) for MNA Monoclinic crystal at different optical frequency.

WAVELENGTH (Angstroms)	THICKNESS (Angstroms)
5000	2772
5500	3027
6000	3538
6500	4593
7000	4663
7500	5254
8000	5649
8500	5823
9000	6670
9500	7760
10000	7899
10500	8526
11000	9697
11500	9918
12000	10010
12500	10010
13000	10010

τe_i, for the same molecule if the interaction occurs in extraordinary direction of polarization. The whole retardation times for *m* molecules aligning inside the crystal (with the length of "L") will be obtained as follows:

$$To = \frac{no.L}{C_o} = \frac{L}{C_o} + \sum_m \tau o_i \qquad (10)$$

$$Te = \frac{ne.L}{C_o} = \frac{L}{C_o} + \sum_m \tau e_i \qquad (11)$$

The final phase difference between these two components (named phase retardation) will be:

$$\Delta\phi = W.(To - Te) = \Sigma W.(\tau o_i - \tau e_i) \qquad (12)$$

IV. MOLECULAR LINEAR PERTURBANCE

In this research, we've approximated the position probability of π-electrons of MNA is space with an elliptical model centering the positive charges of molecule in one of the focal points of an ellipse (with

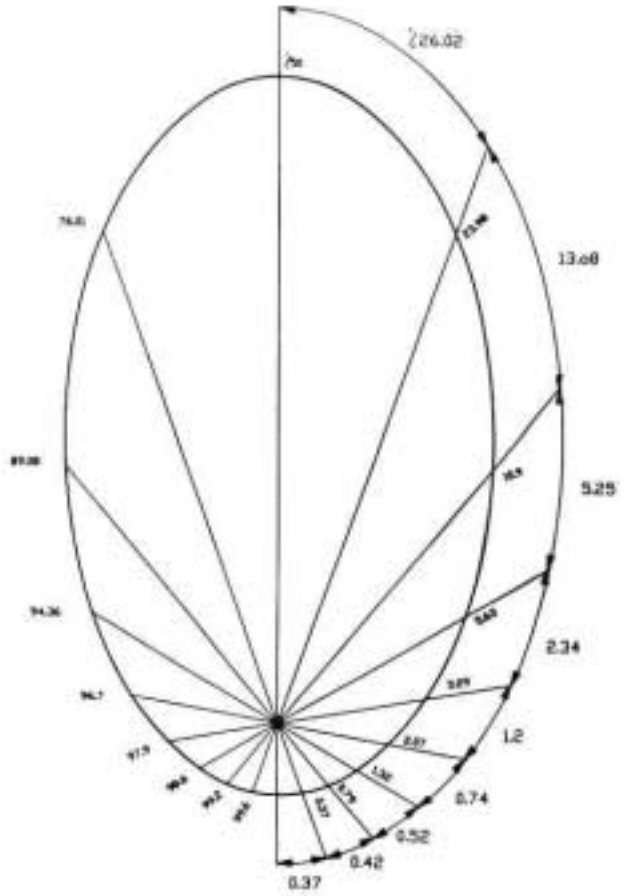


Figure 5. In elliptic model, it has been assumed that the positive charge of molecules are located in one of the focal points and π-electrons cloud in it's elliptical orbit.

distinct eccentricity and π-electrons cloud in it's orbit (Figure 5).

It's shown that the probability of finding electron around the positive center in the apogee position is more than Its' probability in the perigee position (Figure 6). The probability density function (PDF) of π-electron elliptic orbital have been calculated and plotted (Figure 6). In simulation of pockels effect, it's been assumed that the eccentricity of an ellipse is varied slightly according to variation of external applied electric field.

By applying an external transverse electric field to "MNA" crystal (in the range of several volts per micron) the shape of π-electrons orbits will be deformed slightly (Figure7).

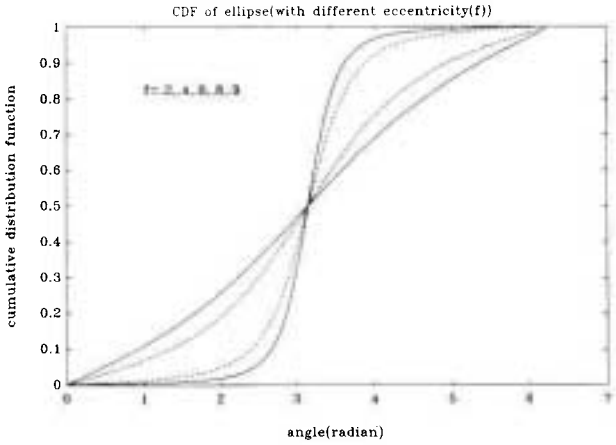


Figure 6. The cumulative distribution function (CDF) of π-electron around the positive center have been plotted in this diagram.

We would expect some noticable variations in microscopic delay parameters (τo_i & τe_i) in case of applying external field. The simulation results have determined the expected linear variation of phase retardation (related to τo_i & τe_i) in terms of electric field.

CONCLUSION

The proposed physical model in this paper which is based on wave-particle nature of photons (photonic treatment) can provide a powerful tool for analysis and design of an organic optical switch. As can be seen in Figure 1 the junction capacitance of quantum

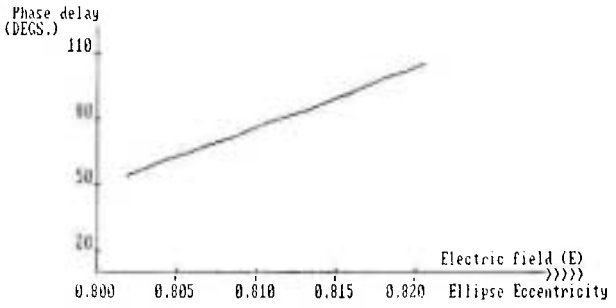


Figure 7. Montecarlo simulation of linear Electro-optic. Pockels effect for MNA Monoclinic crystal (thickness = 5 microns).

film switch is:

$$C = \epsilon_o \frac{W.L}{d} \qquad (13)$$

which will be in the range of femtofarad with the assumption of L < 200 microns, W < 10 microns and d < 1 micron, so that the switching speed will be in the range of about 100 gigabits per second.

High speed data transmission with minimum power dissipation are the main advantages of this organic optical switch. In addition, because of it's wide optical bandwidth these kinds of switchs can transmit data at many different wavelength which will be received by different narrow optical band channels.

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