TECHNICAL DIGEST

PHOTOREFRACTIVE MATERIALS EFFECTS AND DEVICES

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CARRIER AND CHARGE DYNAMICS DURING PHOTOREFRACTIVE RECORDING.

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1. Introduction

Photorefractive processes [1] are described within the framework of the material rate equations based on standard semiconductor physics [2]. Analytical solutions cannot be obtained for high modulation depth m. Numerical solution of these equations is generally acomplished by using a truncated Fourier expansion for all physical magnitudes (carrier and donor concentrations and space charge field). Moreover, it is commonly assumed that the free carrier concentration is small in comparison with the donor and acceptor modulation. This procedure has been shown to yield reasonable agreement with most experiments performed under continuous excitation [3-6].

An alternative approach is to solve numerically the equations without Fourier expansion. As far as we know, only a reduced number of papers have solved numerically the material rate equations successfully using this approach [7,8]. Therefore, it appears appropiate to explore its potentialities and exploit possible advantages on the Fourier expansion approach.

The purpose of this paper is to investigate the kinetics of the photorefractive recording in the highly nonlinear regime (high modulation depth m), by using the method of lines with a finite element collocation procedure (in Refs. [7,8] a finite difference method is used instead).The complete recording curves and spatial profiles have been compared to those obtained by using a limited number of harmonics, so that the value of a truncated Fourier expansion (generally used) can be adequately evaluated.

2. Theoretical Model

We assume that the light intensity pattern is of the form:

$$I = I_o [1 + m \cos(Ky)] \qquad (1)$$

where $K = 2\pi/\Lambda$ (Λ is the light grating period), m is the modulation depth. The electric field is applied along y.

Following the band transport model, the response of the photorefractive material without the photovoltaic effect, is well described by the equations :

$$\partial N^+/\partial t = (sI + \beta)(N - N^+) - \gamma n N^+ \qquad (2)$$
$$\partial n/\partial t = \partial N^+/\partial t + \partial(D\partial n/\partial t + \mu n E)/\partial y \qquad (3)$$
$$\partial(\varepsilon\varepsilon E)/\partial y = e(N^+ - N_A^- - n) \qquad (4)$$

where the motion of carriers is along y and the total concentration of traps is **N**, the concentration of donors at any instant is N^+. The variable **n** is the electron concentration, N_A is the initial number of acceptors, μ is the electron mobility and **D** is the diffusion coefficient. The total electric field is **E** and it is given by the sum of the applied electric filed, E_a, and E_{sc}, which is the space charge field. The dielectric constant is ε, ε_0 is the permittivity of free space, β is the thermal ionization rate and γ refers to the trapping coefficient, the photoionization cross section is **s**. The temperature is **T**.

Poisson's equation (Eq. (4)) can be rewritten, after taking a derivative with respect to time, using the continuity equation and integrating with respect to variable y, as:

$$\partial(\varepsilon\varepsilon_0 E)/\partial t = -eD\partial n/\partial t - e\mu nE + J_0 \qquad (5)$$

where J_0 is a constant independent of the variable y, but it is a function of time.

The boundary condition corresponding to the constraint of a constant aplied voltage is:

$$V = \int_0^L E(y,t)dy \qquad (6)$$

where L is the crystal length.

Assuming periodicity in the grating vector direction, we can express the condition given by Eq. (6) over one grating period of length (Λ) and then, using Eq. (5), we can find J_0 . This function of time can be expressed (where y' = y/Λ) as:

$$J_0 = \int_0^1 [\, e\mu n(y',t)E(y',t)\,]dy' \qquad (7)$$

3. Numerical methods

The set of non linear partial differential equations we have solved numerically is the parabolic system formed by the equations (2), (3) and (5). Constriction given by Eq. (6) determines the value of J_0 as given by Eq. (7).

We have followed the method of lines, using a finite element collocation procedure, with second degree polynomials, which do not depend on time, for the discretization of the spatial variable y. The approximate solution at any time is a second order polynomial over each subinterval (y_n, y_{n+1}). The coefficients of the terms in the polynomial depend only on time. We impose the conditions of continuity of the polynomial and of its first spatial derivative on each extreme of the subinterval. The number of subintervals we took was dependent on the value of *m*. The larger *m*, the larger the number of subintervals. For *m* = 0.9 we needed 45 subintervals. For *m* = 0.01 only 12 were required to get convergence.

The size of the time intervals we used to update the value of the current density, J, and the corresponding value of J_0 was a small fraction (around 1/200) of the carrier life time (which is $\approx 6 \times 10^{-6}$ sec.), for the initial part of the process (0 to 10^{-4}

sec) and around one half of the carrier life time for the rest of the process, i. e., until reaching the stationary state (after about 2 seconds of total time).

Results

Recording curves for the fundamental grating corresponding to three modulation values (m = 0.3, 0.6, 0.9) have been numerically simulated. Results are similar to those obtained by different authors either by using a truncated Fourier method (6) or a finite-difference approach (7). Oscillations in the grating amplitude appearing for low m (and predicted by the analytical solution of the linearized equations) become smoother and even disappear for high m, in correlation with the behavior observed for the phase.

The number of harmonics contributing to the overall kinetics increases with m. For m = 0.3 three harmonics are sufficient to satisfactorily reproduce the full growth curve, whereas 6 or even 9 are required in the case m = 0.9.

The dependence of the steady-state amplitude on m for the first three harmonics has been determined. The supralinearity, is even more pronounced for the second and third harmonics. The increasing relative contribution of the harmonics with m is well illustrated in figure 1, that also includes the point obtained by Brost (7) for m = 1. The dependence E_1/E_2 vs m follows an $1/m$ law as derived from an analytical perturbative treatment.

The profiles for the donor concentration (or equivalently charge density) are given in figure 2 for the three above m values. They correspond to the steady-state situation and incorporate the contribution of all harmonics. They are markedly non-sinusoidal. In particular, for high m they show a split structure with two prominent maxima. In order to evaluate the adequacy of a truncated Fourier expansion the profiles derived from the contribution of the first 3 and 6 harmonics are shown for comparison in figure 3. At least 6 harmonics are needed for a reasonable (not excellent) agreement with the full profile.

Discussion

It has been confirmed that the method of lines, using a finite element collocation procedure is an useful alternative to that based on the Fourier expansion of the physical magnitudes. The obtained results show that for m = 0.9 at least 6 harmonics are needed for a good reproduction of the full growth kinetics as

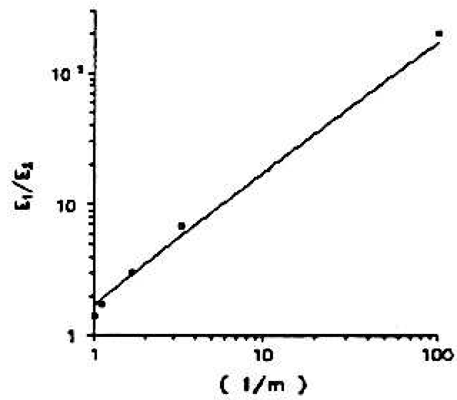

Fig. 1.- Log - log plot of the ratio E_1 divided by E_2 *Vs.* (1/m). The best fit is $(E_1/E_2) = 1.73*(1/m)$ and is the continuos line. The small squares are the calculated values.

well as of the charge profile. This is in agreement with the conclusions based on elaborated convergence criteria using the truncated Fourier method [6].

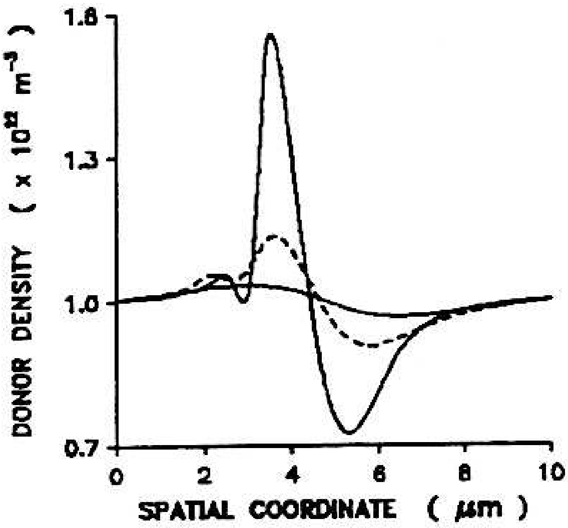

Fig. 2.- Profile of donor concentra - tion;---:for m=0.3, — — —:for m=0.6, ——— :for m=0.9.

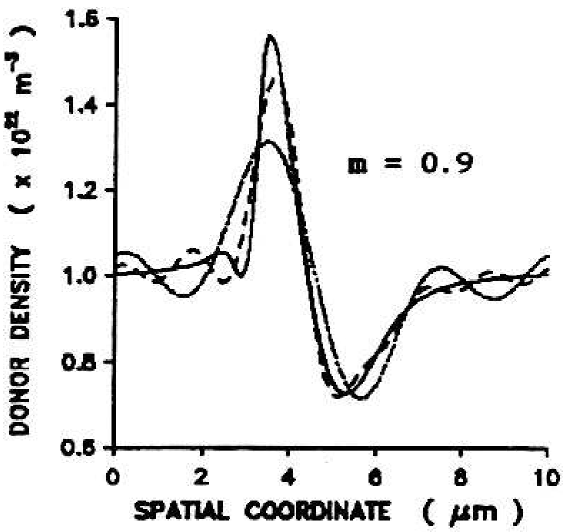

Fig. 3.- Profile of the donor concentration. Total concentration:——; with 3 harmonics:----; with 6 harmonics:— — —.

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