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# Modelling of holographic formation of diffraction structures in photopolymerizable compositions

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#### Abstract

In this work the theoretical model of holographic recording of one-dimensional transmission diffraction structures in photopolymerizable compositions is developed. This model is taking in to account the statistical possibility of the fact that, firstly, different processes of polymeric chain growth and termination are taking place simultaneously and, secondly, the non-linear Fabri-Perot interferometer, formed in the sample, causes recording beam intensity oscillations. The correspondence between the theoretical model and experimental data is also shown.

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Keywords: photopolymerization; photopolymerizable materials; diffraction structures

#### 1. Introduction

The experimental study of the kinetics of formation of diffraction structures (DS) in the photopolymerizable materials (PPM) shows one or more local extremums of the diffraction efficiency (Kwon et al. (1999), O'Neill et al. (2002)) and fast oscillations of recording beams' intensity at the sample output (Gleeson et al. (2005)).

First effect can be explained by the simultaneous occurrence of different processes of the polymeric chains growth and termination, for example, by addition the individual radical and by coupling the growing polymeric chains. Each of these processes takes place at its own rate, is characterized by its own ratio of characteristic

\* Sergey Sharangovich. Tel.: +7(3822)41-36-43. *E-mail address:* shr@tusur.ru polymerization and diffusion times and, therefore, has its own kinetics. Accounting each of these processes will allow to more fully describe the DS recording process. Known theoretical models take into account the different processes of growth and termination of growing polymeric chains, however, they describe only a numerical solution of the recording problem. (Li et al. (2014)).

Second effect in Gleeson et al. (2005) is explained by the incident recording beams intensity variations and mechanical vibrations of experimental setup. We suppose that this effect can be explained by formation the non-linear Fabri-Perot interferometer in the sample, the non-linearity of which is due to refractive index changing caused by the DS recording process.

The aim of this work is to obtain analytical solution of holographic recording of one-dimensional transmissive diffraction structures problem, taking in to account the statistical possibility of the fact that, firstly, different processes of polymeric chains growth and termination are taking place simultaneously and, secondly, the non-linear Fabri-Perot interferometer with refractive index changing is causing the recording beams intensity oscillations.

#### 2. Theoretical model for many formation processes

General kinetic equations of diffraction structures holographic formation in photopolymers are the base of theoretical model being developed:

$$\frac{\partial M}{\partial t} = \operatorname{div}\left(D_m \operatorname{grad} M\right) - \frac{K_g \cdot K_b^{-k}}{\left[\alpha_0 \beta < K > \tau_0 / (1/\tau_0 + \beta M)^k\right]} \cdot \left[I(\mathbf{r}, t)\right]^k M^h,$$
(1)

$$\frac{\partial n}{\partial t} = \delta n_p \cdot \frac{K_g \cdot K_b^{-k}}{\left[\alpha_0 \beta < K > \tau_0 / (1/\tau_0 + \beta M)^k\right]} \cdot \left[I(\mathbf{r}, t)\right]^k \frac{M^h}{M_n} + \delta n_i \operatorname{div}(D_m \operatorname{grad} \frac{M}{M_n}),$$
(2)

where  $D_m$  – diffusion coefficient;  $\delta n_p$  and  $\delta n_i$  characterize the refractive index changing due to photopolymerization and diffusion processes respectively;  $K_g$ ,  $K_b$  – coefficients of polymer chain growth and termination respectively;  $\alpha_0$  – absorption coefficient of the dye;  $\beta$  – photoinitiation reaction parameter;  $\langle K \rangle$  – concentration of the dye;  $\tau_0$  – the lifetime of the dye molecule excited state;  $M_n$  – initial monomer concentration; k – formation process non-linearity coefficient;  $I(\mathbf{r}, t)$  – recording interference pattern.

Solutions of the equations (1) and (2) will be found in the following form:

$$M(\tau, y) = M_0(\tau, y) + \sum_{j=1}^{B} M_1^j(\tau, y) \cdot \cos(\mathbf{K} \cdot \mathbf{r}),$$
(3)

$$n(\tau, y) = n_0(\tau, y) + \sum_{j=1}^{B} n_1^j(\tau, y) \cdot \cos(\mathbf{K} \cdot \mathbf{r}), \qquad (4)$$

where j = 1...B – number of polymeric chain termination process;  $M_0(\tau, y)$  – zeroth harmonic of monomer concentration,  $M_1^j(\tau, y)$  – first harmonics of monomer concentration for each process;  $n_0(\tau, y)$  – zeroth harmonic of refractive index,  $n_1^j(\tau, y)$  – first harmonics of refractive index for each process; **K** – grating vector, **r** – radius-vector.

Using methodic from Dovolnov, Sharangovich (2005) we will write the expression for the zeroth harmonic of monomer concentration and refractive index:

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