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A. Veltri [a] , R. Caputo [a] , L. De Sio [a] , C. Umeton [a] & A. V. Sukhov [b]

[a] Liquid Crystal Laboratory-LICRYL, National Institute for the Physics of Matter of the National Council of Rsearches (INFM-CNR), Centro di Eccellenza per Materiali Innovativi Funzionali in Calabria-CEMIF.CAL, Department of Physics-University of Calabria, Rende (CS), Italy

[b] Institute for Problems in Mechanics, Russian Academy of Science, Moscow, Russia

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Theoretical Characterization of the Holographic Recording of Diffraction Grating in Multicomponent Media

A. Veltri
R. Caputo
L. De Sio
C. Umeton
Liquid Crystal Laboratory–LICRYL, National Institute for the Physics of Matter of the National Council of Rsearches (INFM-CNR), Centro di Eccellenza per Materiali Innovativi Funzionali in Calabria-CEMIF.CAL, and Department of Physics-University of Calabria, Rende (CS), Italy

A. V. Sukhov
Institute for Problems in Mechanics, Russian Academy of Science, Moscow, Russia

We report simulations of a theoretical model describing the formation of holographic diffraction gratings in multicomponent materials. The concentration of the chemical species in the initial mixture plays a fundamental role in determining the final features of the realized sample; our investigation is devoted to determine the best initial mixture realizing good holographic gratings. Along with the model, that is valid for any initial the multicomponent mixture, we report a complete characterization of the numerical solution of the model for two well known cases: H-PDLC and POLICRYPS grating. Obtained results are in good agreement with experimental observation, showing that our model represent a necessary reference for fabrication and the characterization of holographic diffraction gratings in multicomponent materials.

Keywords: diffraction gratings; liquid crystals; polymers

Address correspondence to A. Veltri, Liquid Crystal Laboratory–LICRYL, National Institute for the Physics of Matter of the National Council of Rsearches (INFM-CNR), Centro di Eccellenza per Materiali Innovativi Funzionali in Calabria-CEMIF.CAL and Department of Physics-University of Calabria, Rende (CS) I-87036, Italy. E-mail: aveltri@fis.unical.it

INTRODUCTION

A well known technique used for fabrication of diffraction gratings in multicomponent media is based on an inhomogeneous polymerisation effect, photo-induced by the interference pattern of two intersecting laser beams [1,2]. The realization of such devices in polymeric-liquid crystalline composite materials allows to implement their features. Indeed, the application of an external voltage introduces the possibility of modulating the diffraction efficiency of the grating. The utilized fabrication process, referred to as *"laser curing"* leads, in general, to the formation of a grating consisting in a sequence of polymeric slices alternated to films of Polymer Dispersed Liquid Crystal (PDLC) droplets. Although the Diffraction Efficiency (DE) of this kind of samples can be quite good, the grating reveals either high scattering losses (when the droplet size is comparable with the wavelength of the impinging radiation) or rather high values of the switching voltage (in the opposite case). These drawbacks spoil, in general the performance of devices based on PDLC gratings. Recently, a different approach to the realization of Liquid Crystal (LC) based holographic gratings has been realized, with the fabrication of the so called POLICRYPS (POlymer LIquid CRYstal Polymer Slices) grating [3–7].

In this article, we present a numerical model developed in order to characterize the behaviour of the DE (the main feature of diffraction gratings) as a function of the initial concentration of the non photosensitive chemical species. We also present the solutions of this model obtained by adopting, for boundary conditions, the experimental conditions commonly utilized for realizing these devices.

THEORETICAL MODEL

In order to depict the grating fabrication process, we have used a detailed chemical diffusive model for the formation of structures in liquid crystalline composite materials [5] and we have solved it in the case of different initial concentration σ_0. of liquid crystal. In this case, the system of coupled equations that govern the whole process is given by

$$\frac{d\mu}{d\tau} - B\frac{\partial}{\partial\xi}\left[(1-\nu)^{\frac{2}{3}}\frac{\partial}{\partial\xi}\left(\frac{\mu}{1-\nu}\right)\right] + (1+m\sin\xi)^{\frac{1}{2}}\mu = 0 \tag{1}$$

$$\frac{d\nu}{d\tau} - \frac{G}{2}(1+m\sin\xi)\left[N_0^2(1-\gamma) + N_0(1+\gamma) + \frac{2\gamma}{1-\gamma}\right]\gamma^{N_0} = 0 \tag{2}$$

$$\frac{d\sigma}{d\tau} - B\frac{\partial}{\partial\xi}\left[(1-\nu)^{\frac{2}{3}}\frac{\partial}{\partial\xi}\left(\frac{\sigma}{1-\nu}\right)\right] = 0 \tag{3}$$

where σ, μ and ν are the normalized concentration of LC, free monomers and polymerised monomers respectively; N_0 stands for the least number of monomer molecules which are needed for the formation of an immobile polymer chain. We have introduced a dimensionless coordinate $\xi = 2\pi x/\Lambda$ (Λ is the fringe spacing), a dimensionless time $\tau = [k_p/k_t (k_t g W I)^{\frac{1}{2}}]$t.B, G and γ are defined as:

$$B = \frac{4\pi D k_t^{\frac{1}{2}}}{(gW_0 I)^{\frac{1}{2}}\Lambda^2} \quad G = \frac{(gW_0 I k_t)^{\frac{1}{2}}}{k_p T} \quad \gamma = \frac{\mu}{\mu + G\sqrt{(1 + m\sin\xi)}}.$$

where t is the time, I is the initiator concentration, k_p and k_t are the chemical prolongation and termination constants for the polymer formation reactions, g represents the activation probability of the initiator molecules when acted on by the radiation; D is the monomer diffusion constant; $W_0 = I_1 + I_2$ with $I_1 = E_1\, E_1^*$ and $I_2 = E_2\, E_2^*$ intensities of the two interfering beams; m is the visibility of the fringes. Parameters B and G are related to diffusivity and curing intensity respectively, while, the variable γ has been introduced only to enhance the readability of equations.

NUMERICAL SOLUTIONS

Equations (1)–(3) represent a time dependent, non liner system which can be solved only by means of the numerical scheme described elsewhere [5,6]. As a reference for discussion of results, we use Figure 1: the modulation $\Delta\sigma$ of the liquid crystal concentration across the fringes, calculated from from the steady state solution of system (1)–(3), as the first Fourier component of $\sigma(\xi)^{[5]}$, is represented in the B-G plane. This variable determines the DE of gratings and therefore we believe that the two maxima which are presented in Figure 1 identify the two different regimes corresponding to the formation of good H-PDLC and POLICRYPS gratings. In order to determine the best initial mixture for H-PDLC formation we have choose $B = 0.5$ and $G = 0.5$; results of this characterization are presented in Figure 2, where $\Delta\sigma$ is reported as a function of initial value σ_0.

In this case, we are in the conditions that, very probably, will produce an H-PDLC grating. Results presented in Figure 2 show a maximum around an initial mixture of 40% of liquid crystal. By repeating the same characterization for $B = 2.17$ and $G = 0.08$, we obtain results reported in Figure 3. In this case it is possible to see that the maximum is higher and is shifted to about $\sigma_0 = 0.3$. These results are consistent with experiments. In Figure 3 it is also possible to see a secondary maximum around $\sigma_0 = 0.9$, which is due to the fact that, by increasing the LC initial

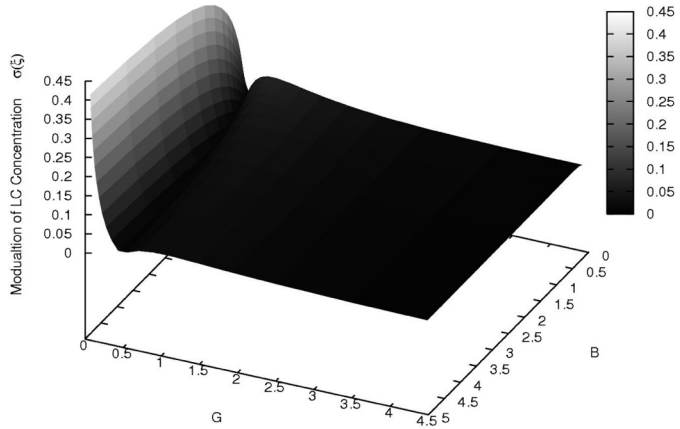

FIGURE 1 The Modulation $\Delta\sigma$ of the LC concentration is presented as a function of parameters B and G in a 3D surface. The smooth maximum identifies the H-PDLC grating zone while the asymptotic zone on the left identifies the POLICRYPS gratings formation.

concentration, we will produce H-PDLC gratings also in this BG-point; this way we have $\Delta\sigma = 0$ passing from a regime to another. The curing process is highly dependent on the initial concentration, which can be considered the third parameter governing the system.

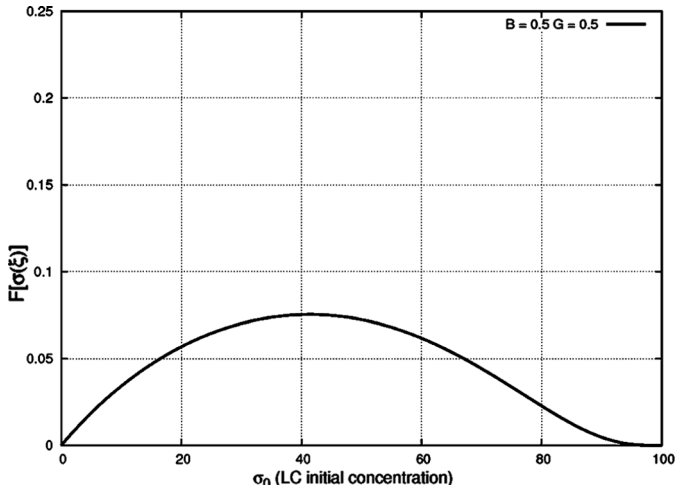

FIGURE 2 The Modulation $\Delta\sigma$ of the LC concentration is presented as a function of the initial LC concentration σ_0 in a particular point of the BG plane, (B = 0.5 and G = 0.5).

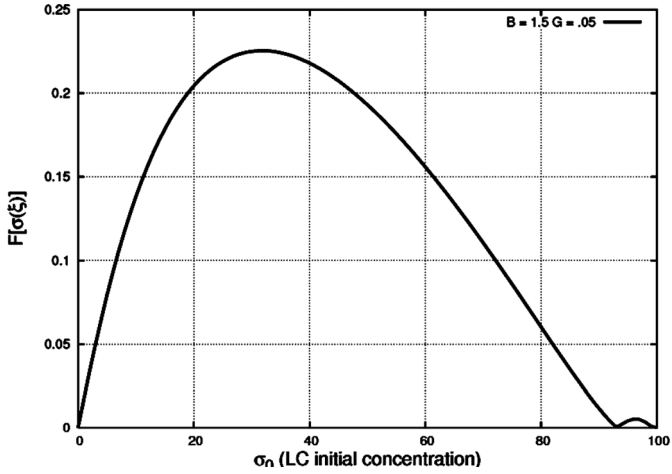

FIGURE 3 The Modulation $\Delta\sigma$ of the LC concentration is presented as a function of the initial LC concentration σ_0 in the point B = 2.17 and G = 0.08 of the BG plane.

CONCLUSIONS

When dealing with applied physics from a theoretical point of view, one of the targets of the work is to give indications, as precise as possible, to realize new technologies or to improve the existing ones. In this article we report solutions obtained from a model developed for the characterisation of the behaviour of the DE as a function of the initial concentration of the guests chemical species. The photochemical-diffusive model, through the BG-surface, gives interesting information in term of curing intensity and temperature, about the "know how" for the fabrication of good POLICRYPS gratings or eventually good H-PDLC ones. A further information, however, can be of interest as well. In particular, it is useful to know what is the best initial condition of the utilized mixture. Solutions offered by our model are in accordance with different experimental conditions.

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