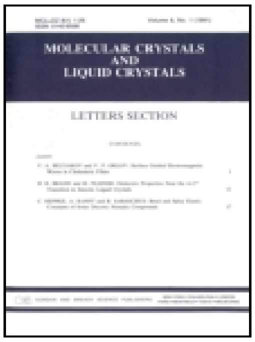


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# Impact of Doping CdSe/ZnS Quantum Dots on the Elasticity Coefficients of Nematic

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*C-V dependencies of pure NLC cells and suspensions with semiconductor CdSe/ZnS QDs were simulated. Comparison method of fitting theoretical capacity-voltage dependencies with experimental data of homogeneously aligned by polyimide layers LC cells was applied to estimate elasticity coefficients for splay and bend director deformation and parallel and perpendicular components of NLC cell dielectric constant. Increase of these parameters for QDs-NLC suspension compared to pure NLC was observed when the QDs concentrations were 0.5–1 mg/ml. The calculations were performed excluding the screening effect associated with QDs doping which can increases Frederick's threshold voltage.*

**Keywords** Nematic liquid crystal; quantum dots; capacitance; elasticity coefficients; dielectric constant

## Introduction

Frank elasticity coefficients $K_{11}$, $K_{22}$, $K_{33}$ characterize splay, twist and bend deformations of nematic liquid crystals (NLC) and have a profound impact on electro-optic effects. Selection of liquid crystal mixture with specific elasticity coefficients is vital for development of liquid crystal devices as elasticity coefficients affect Frederick's threshold voltage and dynamic of LC's optical response.

Nanoparticle doping in LC causes decrease in order parameter that influences $K_{ii}$ and dielectric anisotropy alternation of suspension in comparison with pure NLC [1]. Doping NLC with CdSe quantum dots (QDs) caused decrease of threshold voltage and elasticity coefficient $K_{11}$ as the size of the nanoparticles is reduced [2]. As concentration rises from 0.1 to 0.2 wt% of CdSe/ZnS core-shell QDs, phase delay decrease was observed along with voltage threshold and effective dielectric permittivity decrease, what is the evidence of director's pretilt angle increase [3].

In article [4] to determine elasticity coefficients of homogeneous and homeotropic NLC was applied a method, based on numeral computation of balance equations in NLC volume and on surface and further fitting of calculated NLC cell capacitance to applied voltage (C-V) dependencies to match experimental data.

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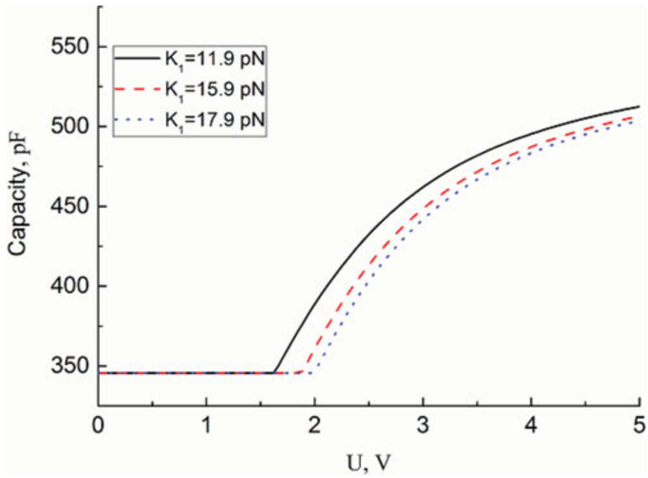


**Figure 1.** Simulated C-V dependencies of homogeneous NLC cell for splay deformation elasticity coefficients 11.9 pN, 15.9 pN and 17.9 pN, in the event of $\theta_0 = 0°$.

Main goal of this article is the investigation of possibility of elasticity coefficients determination of NLC and CdSe/ZnS suspension using simulation of C-V dependency. In this article C-V dependencies of homogeneous NLC cells with positive dielectric anisotropy doped with QDs are simulated. Impact of elasticity coefficients $K_{11}$ and $K_{33}$ and director's pretilt angle on C-V dependencies are investigated by comparison of experimentally achieved dependencies with simulated ones. The elasticity coefficients, dielectric permittivity components and director's pretilt angle are determined.

## Simulating of NLC Capacity to Applied Voltage Dependencies

Free energy minimization results in balance equations, which depends on director **n** distribution, that acts as function of spatial coordinates and their derivatives according to the static theory. Solving of these equations with the lowest free energy provides physically possible director **n** distribution [5]. In case of planar orientation director's pretilt angle's $\theta$ value as function of $z$ can be obtained by numerical calculation of equation:

$$z\frac{2}{d}\int_{\theta_0}^{\theta_m}\left(\frac{\left(1+\kappa\sin^2\hat{\theta}\right)\left(1+\gamma\sin^2\hat{\theta}\right)}{\sin^2\theta_m-\sin^2\hat{\theta}}\right)^{\frac{1}{2}}d\hat{\theta}$$

$$=\int_{\theta_0}^{\theta}\left(\frac{\left(1+\kappa\sin^2\hat{\theta}\right)\left(1+\gamma\sin^2\hat{\theta}\right)}{\sin^2\theta_m-\sin^2\hat{\theta}}\right)^{\frac{1}{2}}d\hat{\theta}. \quad (1)$$

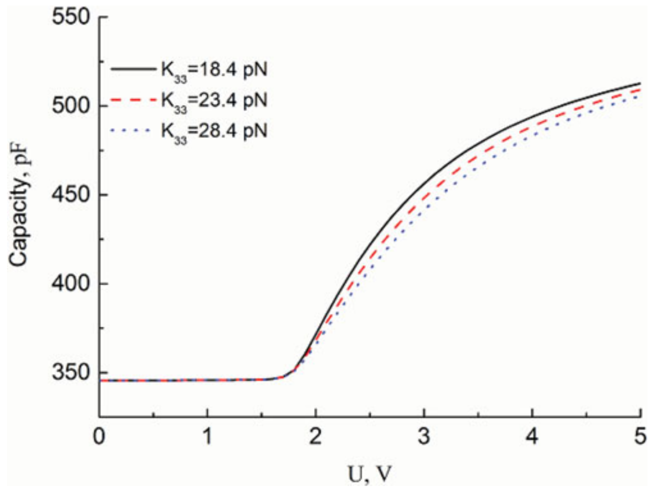


**Figure 2.** Simulated C-V dependencies for bend-deformation elasticity coefficient $K_{33}$ 18.4 pN, 23.4 pN and 28.4 pN

Supposing that at the interphase boundaries director is situated in plane of plates, in other words $\theta(0) = \theta(\mathrm{d}) = \theta_0 = 0^\circ$, Frederick's threshold voltage for splay deformation is

$$U_{th} = \pi\sqrt{K_{11}}\Big/\sqrt{\varepsilon_0\Delta\varepsilon}, \tag{2}$$

where $\varepsilon_0$ is electric constant, $\Delta\varepsilon = \varepsilon_\parallel - \varepsilon_\perp$ is dielectric anisotropy. Therefore, elasticity coefficient $K_{11}$ can be calculated as

$$K_{11} = U_{th}^2\varepsilon_0\Delta\varepsilon\big/\pi^2. \tag{3}$$

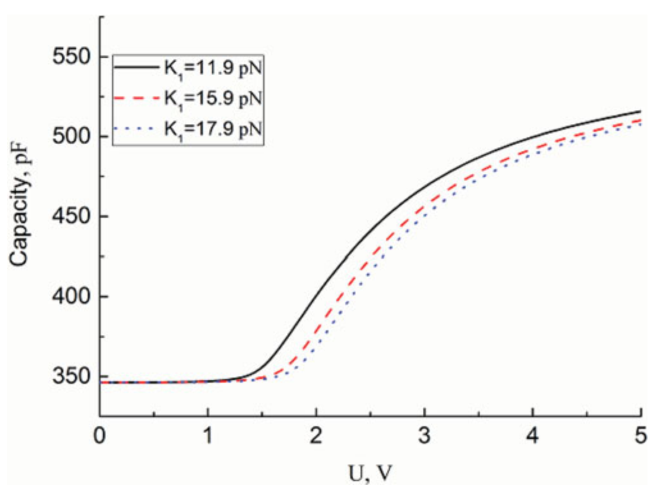


**Figure 3.** Simulated C-V dependencies for pretilt angle $\theta_0 = 3^\circ$.

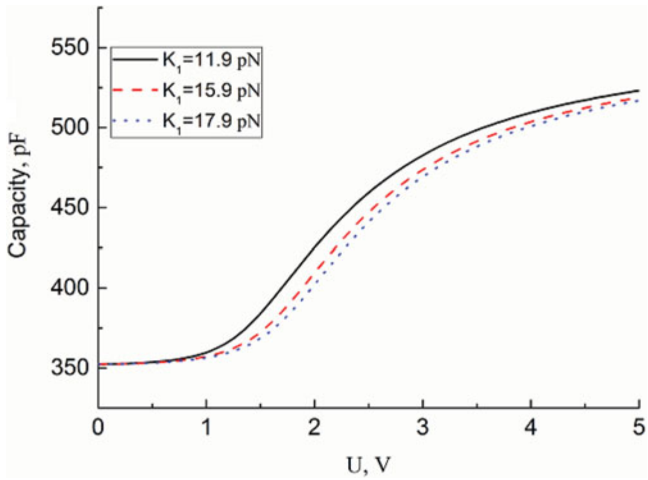


**Figure 4.** Simulated C-V dependencies for pretilt angle $\theta_0 = 10^\circ$.

Simulated C-V dependencies of homogeneous cell 22 $\mu$m in thickness and with plates $1.13 \cdot 10^{-4}$ m$^2$ in area for three values of splay deformation elasticity coefficient $K_{11}$ are shown on Fig. 1. The following parameters were used for simulation: $\theta_0 = 0^\circ$, $K_{33} = 18.4 \cdot 10^{-12}$ pN, $\Delta\varepsilon = 5$, $\varepsilon_\perp = 7.6$. Increase of elasticity coefficient $K_{11}$ correlates with increase of Fredericks threshold.

Threshold voltage observed in experiment can differ from its simulated value for a number of reasons. Its increase can be caused by impact of screening effect, which depends on dielectric permittivity and thickness of LC and alignment layers [6]. Impact on threshold voltage and director's pretilt angle in different alignment layers was shown in [7].

Simulated C-V dependencies for three values of bend-deformation elasticity coefficients $K_{33}$ are shown on Fig. 2. Increase of elasticity coefficient $K_{33}$ causes decrease of cell capacity, which emerges in altering dependency's curvature.

Insignificant increase of NLC director's pretilt angle can noticeably alter elasticity coefficient $K_{11}$ measurement, which is related with decrease of threshold voltage in experimental dependency. C-V dependencies for pretilt angles 3° and 10° are shown on Figs. 3, 4.

As shown on Fig. 4 increase of director's pretilt angle for same elasticity coefficients causes less prominent threshold. Therefore increase of pretilt angle caused by doping NLC with nanoparticles must be taken into consideration. Effective dielectric anisotropy of NLC cell on appliance of external electric field depends on director's distribution in NLC volume

**Table 1.** NLC cells parameters

| No cell | Cell thickness, $\mu$m | QD concentration, mg/ml |
|---|---|---|
| 1 | 7,1 | — |
| 2 | 13.2 | 0.5 |
| 3 | 13.4 | 1 |

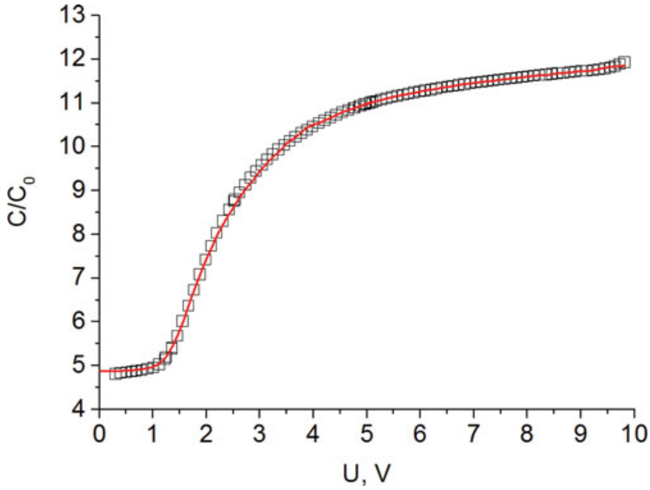


**Figure 5.** Experimental (squares) and simulated (solid line) NLC cell No 1 C-V dependency.

and can be equated as

$$\varepsilon\left(z\right)=\varepsilon_0\left[\varepsilon_\perp+\Delta\varepsilon cos^2\theta\left(z\right)\right]. \tag{4}$$

Therefore NLC cell capacity is

$$C=\frac{S}{\int_0^d\frac{1}{\varepsilon(z)}dz}. \tag{5}$$

Taking into account correlation of NLC director's distribution and effective dielectric permittivity, elasticity coefficients can be fitted theoretical calculations. Fitting of experimental C-V dependency to theoretical curve can be achieved by variation of elasticity

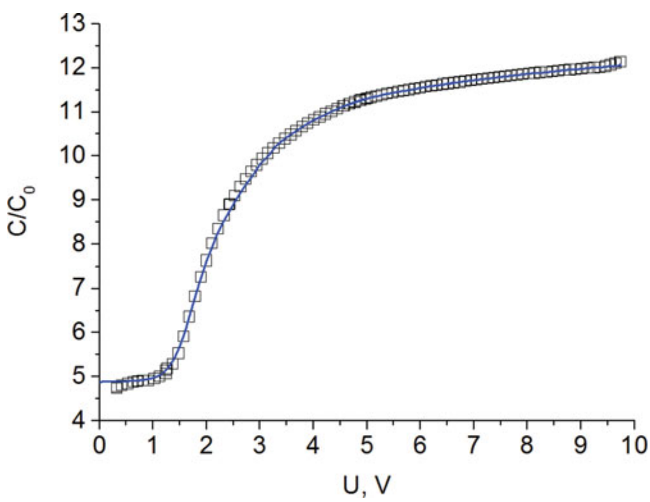


**Figure 6.** Experimental (squares) and simulated (solid line) NLC cell No 2 C-V dependency.

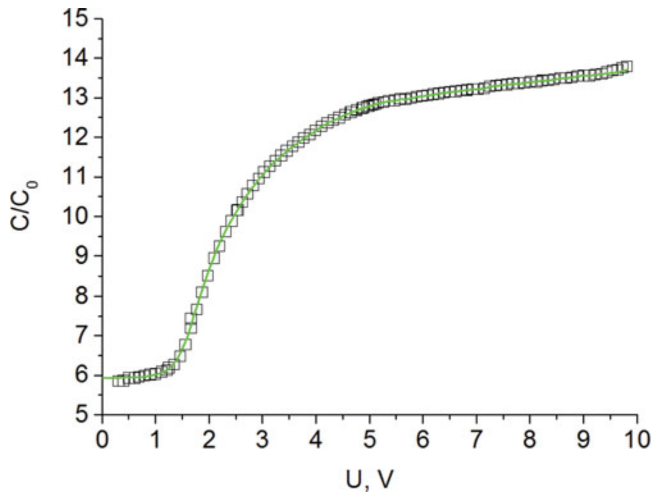


**Figure 7.** Experimental (squares) and simulated (solid line) NLC cell No 3 C-V dependency.



coefficient's values. Thus, dielectric permittivity components can be determine and estimate influence on them nanoparticles doping.

## Results of Fitting Experimental and Theoretical Data and Discussion

The developed method was used to investigate parallel-sided LC cells assembled from two glass plates, covered with conductor layer, based on indium and tin oxides, and polyimide alignment layer. Cells were filled with pure LC-1282 (Niopic, Moscow) and its suspension with semiconductor core-shell QDs CdSe/ZnS 3.5nm in core size (Table 1). Suspension was created by adding dry shots of 0.5 and 1 mg/ml QDs into nematic LC mesophase. Before filling LC/QDs suspensions were stirred by ultrasonic bath for 1.5 hours. C-V dependency was measured by applying of 1 kHz sine current with specially developed computer program.

Mathematical simulation of C-V dependences of these cells were performed. For each cell C-V dependencies were fitted with experimental data as shown on Figs. 5–7.

Calculated values of elasticity coefficients, dielectric permittivity components and pretilt angle of investigated NLC cells, obtained by fitting simulated and experimental curves, are listed in Table 2.

Data obtained by simulation shows that with increase of QDs concentration increase of parallel and perpendicular components of dielectric permittivity and decrease of elasticity coefficient $K_{33}$ are observed. Observed increase of $K_{11}$ elasticity coefficient can be related

**Table 2.** Calculated NLC properties of pure NLC and NLC/QDs suspension cells

| No cell | $K_{11}$, pN | $K_{33}$, pN | $\varepsilon_{\parallel}$ | $\varepsilon_{\perp}$ | Pretilt angle, degree |
|---|---|---|---|---|---|
| 1 | 18 | 7.5 | 15 | 4.8 | 5 |
| 2 | 22 | 4.5 | 16 | 4.8 | 5 |
| 3 | 25 | 5.5 | 17.8 | 5.85 | 5 |

with decrease of effective voltage of electric field in LC volume, which causes overestimation of experimental value of threshold voltage used in simulation. Screening effect caused by semiconductor QDs doping can be the matter of voltage increase. Further investigation of elastic and dielectric properties of NLC suspensions with different semiconductor QDs concentrations is required for interpretation of achieved results.

## Conclusion

C-V dependencies of pure NLC cells and suspensions with semiconductor QDs were simulated. It was shown that elasticity coefficients for splay- and bend-deformation and parallel and perpendicular components of dielectric constant of NLC cell can be derived by fitting the calculated C-V dependence with the experimental curves. The obtained results show that screening effect and semiconductor nanoparticle doping must be considered as they cause overestimating of the threshold voltage value, used in simulation. Further studies with semiconductor NLC/QDs suspensions will assess the impact of these factors and improve the accuracy of properties calculating of such systems through simulation.

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