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Light-Scattering by Small Solid Spherical Particles Dispersed in a Nematic Cell

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The light scattering differential cross-section by small identical spherical particles in nematic liquid crystal is numerically calculated at the infinitely rigid director anchoring with particles surface. It is taking into account the influence of the correlations between the positions of the particles.

Keywords: light scattering; differential cross-section; filled liquid crystal

INTRODUCTION

Filled liquid crystals consist of the nematic liquid crystal matrix which contains small silica particles. The particles induce the disturbances in the nematic director field that leads to the intensive light scattering. Under the action of electric field the inhomogeneties of the director field decreases and the transparency of the sample increases. Due to this the filled liquid crystals are very perspective for using in display technologies and are intensively studied in the last years^[1-4].

Intensity of the light scattering caused by the director inhomogeneity

around a single particle depends on the liquid crystals elastic properties and on both the director anchoring energy at the particle surface and the particle size. The light scattering in the filled liquid crystals at the weak director anchoring with particle surface has been studied in paper^[5]. In the present paper we continue this investigation and consider the intensity of light scattering in the filled liquid crystals at the infinitely rigid director anchoring with particle surface. In this case the particles can induce disclinations in the director field^[6] that must lead to especially strong light scattering.

THE GENERAL EXPRESSIONS FOR LIGHT SCATTERING CROSS-SECTION

Consider the nematic liquid crystal which contains some concentration of small macroscopic spherical particles having the same radius R. These particles disturb the nematic director field that leads to the scattering of the incident light wave. In Rayleigh-Gans approximation the light scattering cross-section by the director inhomogeneities is given by^[7].

$$\frac{d\sigma}{d\Omega} = \frac{k^4}{16\pi^2} |\vec{e}_{\alpha}\hat{\varepsilon}(\vec{q}_{s})\vec{e}_{\mu}|^2, \qquad (1)$$

where

$$\hat{\varepsilon}(\vec{q}_s) = \iiint \left(\hat{\varepsilon}(\vec{r}) - \hat{\varepsilon}^0\right) e^{-i\vec{q}_s\vec{r}} dV, \qquad \vec{q}_s = \vec{k}' - \vec{k}. \tag{2}$$

Here \vec{e}_{α} , \vec{e}_{μ} are the unit vectors denoting the polarization of the incident and scattered light waves, \vec{k} , \vec{k}' are the wave vectors of these waves, $\hat{\epsilon}(\vec{r})$, $\hat{\epsilon}^0$ are the dielectric susceptibility tensors of the disturbed and undisturbed nematics, respectively. The integration is carried out over the volume of nematics neglecting the small volume occupied by the spherical particles.

Dielectric susceptibility tensor of nematic has the form

$$\varepsilon_{ij}(\vec{r}) = \varepsilon_{\perp} \delta_{ij} + \varepsilon_{a} n_{i}(\vec{r}) n_{j}(\vec{r}), \tag{3}$$

where $\varepsilon_a = \varepsilon_{\parallel} - \varepsilon_{\perp}$ is the anisotropy of dielectric susceptibility at the optics frequencies, \vec{n} is the nematic director.

Assume the particles concentration to be small enough so the regions of director disturbance by different particles do not overlap. Then one can

write

$$\varepsilon_{ij}(\vec{r}) = \varepsilon_{ij}^{0} + \sum_{m} \delta \varepsilon_{ij}(\vec{r} - \vec{r}_{m})\Theta(d - |\vec{r} - \vec{r}_{m}|), \tag{4}$$

where d is the average distance between particles, the function $\Theta(x) = 1$. if $x \ge 0$ and $\Theta(x) = 0$, if x < 0; the summation is over all N particles.

We direct the z-axis of the Cartesian reference system along the director of undisturbed nematic then we have from (3), (4), we have

$$\varepsilon_{ij}^{0} = \delta_{ij}(\varepsilon_{\perp} + \varepsilon_{a}\delta_{iz}),$$

$$\delta\varepsilon_{ij}(\vec{r}) = \varepsilon_{a} \begin{pmatrix} n_{x}^{2} & n_{x}n_{y} & n_{x}n_{z} \\ n_{x}n_{y} & n_{y}^{2} & n_{y}n_{z} \\ n_{x}n_{z} & n_{y}n_{z} & n_{z}^{2} - 1 \end{pmatrix} = \varepsilon_{a}\delta\tilde{\varepsilon}_{ij}(\vec{r}). \tag{5}$$

On substituting the expressions (2), (3) into (1) one can get

$$\frac{d\sigma}{d\Omega} = \frac{k^4}{16\pi^2} N \left| \vec{e}_{\alpha} \delta \hat{\varepsilon}(\vec{q}_s) \vec{e}_{\mu} \right|^2 \left(1 + \frac{1}{N} \sum_{\substack{m,m'\\m \neq m'}} e^{-i\vec{q}_s(\vec{r}_m - \vec{r}_{m'})} \right). \tag{6}$$

Taking into account the definition of the pair correlation function $g(\vec{r})^{[8]}$, the sum in (6) can be written as

$$\frac{1}{N} \sum_{\substack{m,m'\\m \neq m'}} e^{-i\vec{q}_{\mathfrak{s}}(\vec{r}_{m} - \vec{r}_{m'})} = \frac{N}{V} \iiint g(\vec{r}') e^{-i\vec{q}_{\mathfrak{s}}\vec{r}'} dV' = cg(\vec{q}_{\mathfrak{s}}), \tag{7}$$

where c = N/V is the concentration of the particles, $g(\vec{q_s})$ is the Fourier transform of the function $g(\vec{r})$. Then the expression (6) takes the final form

$$\frac{d\sigma}{d\Omega} = \frac{k^4}{16\pi^2} N \varepsilon_a^2 |\vec{e}_\alpha \delta \tilde{\varepsilon}(\vec{q}_s) \vec{e}_\mu|^2 S(\vec{q}_s), \tag{8}$$

where $S(\vec{q_s}) = 1 + cg(\vec{q_s})$ is so-called structure factor which describes the influence on the scattering cross-section of correlations in the particles positions. Here we have used the $S(\vec{q_s})$ calculated in paper^[5] on the base of Percus-Yevick approximation^[9].

Let the wave vector \vec{k} of the incident light to be directed along the z axis and the plane yz to be the scattering plane which contains the vectors \vec{k} . $\vec{k'}$. Then

$$\vec{q}_s = \left(0, k \sin \vartheta, -2k \sin^2 \frac{\vartheta}{2}\right), \quad |\vec{q}_s| = 2k \sin \frac{\vartheta}{2}, \tag{9}$$

where ϑ is a scattering angle.

To calculate $\frac{d\sigma}{d\Omega}$ it is necessary to find the director field configuration $n(\vec{r})$ near the particle. At the infinitely rigid director anchoring at the particle surface this distribution takes the complex form between the radial structure near the particle and the disclination loop of strength "-1/2" at the distance a from the particle surface. It was calculated in the paper^[6] and has the next form

$$\beta(r,\theta) = \theta - \frac{1}{2} \arctan \frac{\sin 2\theta}{1/f(r) + \cos 2\theta},\tag{10}$$

where

$$f(r) = \left(\frac{r}{a}\right)^3 + A + B\frac{r}{a} + Ce^{-r/a},$$

$$A = \frac{R^3}{a^2(a-R)^2} \left[R - a + \frac{a^2}{R^2} (4a - 3R) \left(\frac{a}{R} e^{-R/a} - e^{-1} \right) \right],$$

$$B = \frac{R^3}{a^2(a-R)^2} \left[a - R + (4a - 3R) \left(e^{-1} - e^{-R/a} \right) \right],$$

$$C = -\frac{4a - 3R}{a - R}, \qquad a = 1.25R.$$
(11)

Here $\beta(r,\theta)$ is the angle of director deviation from its undisturbed direction (directed along the z axis); r, θ , φ are the spherical coordinates of point with respect to the centre of the particle. In these designations the director components are

$$n_x = \sin \beta(r, \theta) \cos \varphi.$$

 $n_y = \sin \beta(r, \theta) \sin \varphi.$ (12)
 $n_z = \cos \beta(r, \theta).$

Substituting (12) and expression for $S(\vec{q}_s)$ into (8) and taking into account (10), (11) one can calculate the light scattering cross-section by a system of spherical particles in a nematic under the strong director anchoring at the particles surface.

CALCULATION OF THE CROSS-SECTIONS

Let the incident light wave polarization be along the y axis, e.g. in the plane of scattering. Then one can show that the scattered light wave is polarized in the plane of scattering too.

Consider firstly the light scattering with change of polarization. e.g. the polarization vector of scattered light wave is directed along z axis. Then

 $\delta \tilde{\varepsilon}_{yz}(\vec{q}_s) = \iiint n_y(\vec{r}) n_z(\vec{r}) e^{-i\vec{q}_s \vec{r}} dV =$ (13)

$$=-2\pi R^3\int\limits_{1}^{\infty}dx\,x^2\int\limits_{0}^{\pi/2}d\theta\,\sin\!2\beta(x,\theta)\sin\theta\sin(q_zRx\cos\theta)J_1(q_yRx\sin\theta),$$

where we have used the expressions (12) and have integrated over the asimuth angle φ , $J_1(t)$ is the Bessel function.

If the incident light is polarized along the y axis and the scattered light is polarized along the z axis on substituting the expression (13) into the formula (8) we obtain the following expression for the light scattering cross-section:

$$\frac{1}{N\pi R^2} \left(\frac{d\sigma}{d\Omega} \right)_{vz} =$$

$$=\frac{\varepsilon_a^2}{4\pi}(kR)^4\left(\int\limits_1^\infty dx\,x^2\int\limits_0^{\pi/2}d\theta\,\sin 2\beta(x,\theta)\sin\theta\sin(q_xRx\cos\theta)J_1(q_yRx\sin\theta)\right)^2\times$$

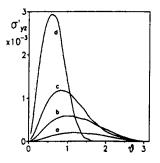


FIGURE 1. Light scattering cross-section with change of polarization σ'_{yz} versus the scattering angle θ at the next values of parameter kR = 1 – a. 1.5 – b. 2 – c. 3 – d.

$$\times S\left(2kR\sin\frac{\vartheta}{2}\right). \tag{14}$$

The quantity $\sigma'_{yz} \equiv \frac{1}{N\pi R^2} \left(\frac{d\sigma}{d\Omega}\right)_{yz}$ versus the scattering angle ϑ is shown in the figure 1 at the different values of the parameter kR. One can compare the results presented in the figure 1 with those obtained for the case of the weak director anchoring at the particle surface^[5]. As it follows from the comparison, the light scattering cross-section at the strong director anchoring is approximately by three orders of magnitude greater than at weak

director anchoring. Besides, in the first case the maximum of the light scattering cross-section is shifted by 10-15 degrees toward the side of the smaller scattering angles and the width of the scattering bands appreciably increases.

To consider the light scattering without change of polarization one has to calculate

 $\delta \tilde{\varepsilon}_{yy}(\vec{q_s}) = \iiint n_y^2(\vec{r}) e^{-i\vec{q_s}\vec{r}} \, dV.$

Similar to the above calculations we get the next expression for the light scattering cross-section when the polarization vectors of the incident and scattered light are directed along the y axis:

$$\frac{1}{N\pi R^2} \left(\frac{d\sigma}{d\Omega} \right)_{yy} =$$

$$= \frac{\varepsilon_a^2}{\pi} (kR)^4 \left(\int_1^\infty dx \, x^2 \int_0^{\pi/2} d\theta \, \sin^2 \beta(x, \theta) \sin \theta \cos(q_x Rx \cos \theta) F(q_y Rx \sin \theta) \right)^2 \times$$

$$\times S \left(2kR \sin \frac{\vartheta}{2} \right), \tag{15}$$

where $F(t) = J_0(t) - J_1(t)/t$.

The results of numerical calculation of $\sigma'_{yy} \equiv \frac{1}{N\pi R^2} \left(\frac{d\sigma}{d\Omega}\right)_{yy}$ versus ϑ are shown in the figure 2.

If the incident light wave is polarized perpendicular to the scattering plane (e.g. along the x axis) the scattered wave has to be polarized only along the same direction as the incident wave. In this case the light scattering cross-section is determined by the Fourier transform

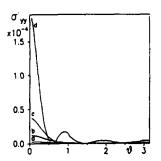
$$\delta \tilde{arepsilon}_{xx}(ec{q_s}) = \iiint n_x^2(ec{r}) e^{-i ec{q_s} ec{r}} \, dV,$$

and takes the form:

$$\frac{1}{N\pi R^2} \left(\frac{d\sigma}{d\Omega}\right)_{xx} =$$

$$= \frac{\varepsilon_a^2}{\pi} \frac{(kR)^4}{(q_y R)^2} \left(\int_1^\infty dx \, x \int_0^{\pi/2} d\theta \, \sin^2\beta(x,\theta) \cos(q_z Rx \cos\theta) J_1(q_y Rx \sin\theta) \right)^2 \times$$

$$\times S\left(2kR \sin\frac{\vartheta}{2}\right). \tag{16}$$



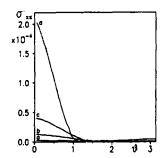


FIGURE 2. Light scattering cross-section without change of polarization σ'_{yy} versus θ at the next values of parameter kR = 1 - a, 1.5 - b, 2 - c, 3 - d.

FIGURE 3. Light scattering cross-section without change of polarization σ'_{xx} versus θ at the next values of parameter kR = 1 - a, 1.5 - b, 2 - c, 3 - d.

In the figure 3 the quantity $\sigma'_{xx} \equiv \frac{1}{N\pi R^2} \left(\frac{d\sigma}{d\Omega}\right)_{xx}$ versus ϑ is shown for some values of the parameter kR. As it is seen from the figures 2, 3 the light scattering cross-section without change of polarization is approximately by one order of magnitude smaller than at the scattering with change of polarization. It is necessary to note that at the weak director anchoring the light scattering cross-section without change of polarization equals zero.

CONCLUSIONS

At the infinitely rigid director anchoring with particle surface the light scattering cross-section with change of light polarization exceeds essentially (by three orders of magnitude) the scattering at the weak director anchoring. The maximum of the scattering cross-section is shitted by 10-15 degrees toward the smaller scattering angles and the width of the scattering light bands increases. Besides, at the infinitely rigid director anchoring the light scattering without change of light polarization takes place. The proper light scattering cross-section is by one order of magnitude smaller than at the scattering with change of light polarization.

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