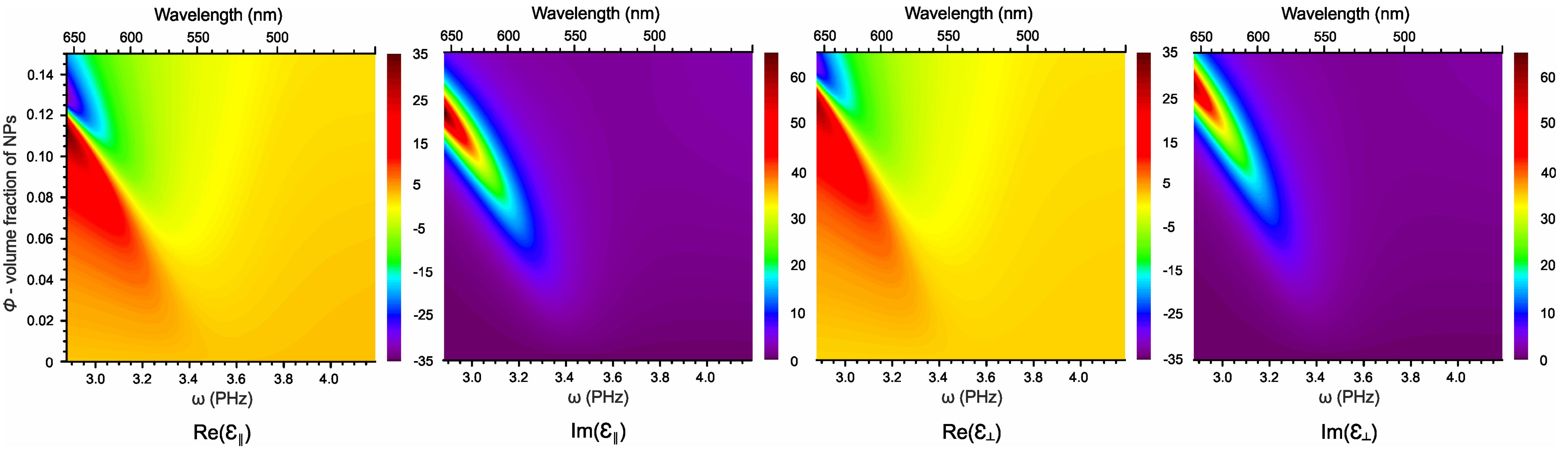
Theoretical description of the optical properties of nematic nanocomposites with gold and silver nanoparticles

Mikhail A. Osipov[1,2*], Alexey S. Merekalov[2] and Alexander A. Ezhov[2,3]
[1] Department of Mathematics and Statistics, University of Strathclyde, Glasgow G1 1XH, Scotland, UK,
[2] Topchiev Institute of Petrochemical Synthesis, Russian Academy of Sciences, 119991 Moscow, Russia
[3] Faculty of Physics, Lomonosov Moscow State University, 119991 Moscow, Russia
E-Mail: m.osipov@strath.ac.uk



The dependence of the real and imaginary parts of the nematic nano-composite (host *5CB* plus AuNPs) on the volume fraction of AuNPs ϕ and cyclic frequency ω

The tensor dielectric constant of the nematic phase doped with NPs

$$(\hat{\varepsilon} - 1)(\hat{\varepsilon} - 1)^{-1} = (1 - \phi)(\hat{\varepsilon}_{LC} - 1)(\hat{\varepsilon}_{LC} + 2)^{-1} + \frac{4\pi}{3}\phi v_{NP}^{-1}\hat{\beta}_{NP}^{eff}$$

v_{NP} – nanoparticle volume

$\hat{\beta}_{NP}^{eff}$ – effective nondimentional polarizability of an NP

ϕ – volume fraction of NPs

Effective polarizability of an NP

$$\alpha_{NP} = a^3\varepsilon_s \frac{\varepsilon_{Me} - \varepsilon_s}{\varepsilon_{Me} + 2\varepsilon_s}$$

a –radius of the NP

Spherical metal NP

Drude model

$$\varepsilon_{Me}(\omega) = 1 - \frac{(\omega_p\tau)^2}{\omega\tau(\omega\tau + i)}$$

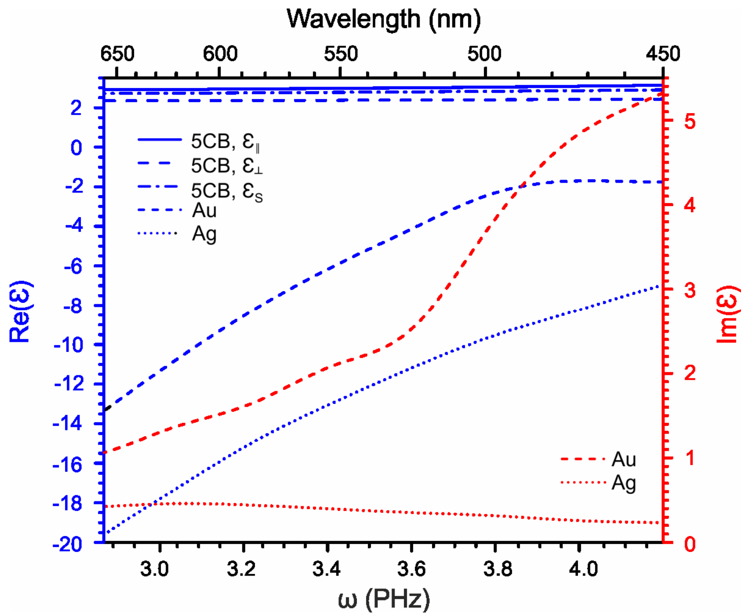
ω_p – metal plasmon frequency

τ – mean free time of electrons

Anysotropic dielectric medium

average susceptibility of the nematic LC

$$\varepsilon_s = \frac{1}{3}(\varepsilon_{\parallel} + 2\varepsilon_{\perp})$$



Frequency dependence of the dielectric constants of gold, silver and the nematic host 4-cyano-4'-pentylbiphenyl (*5CB*)

The longitudinal and transverse components of the dielectric tensor of the nano-composite

$$\varepsilon_{\parallel} = \frac{\left(\varepsilon_{\parallel}^{0} + 2\right)(\varepsilon_{Me} + 2\varepsilon_{s}) + 2\left[(1-\phi)\left(\varepsilon_{\parallel}^{0} - 1\right)(\varepsilon_{Me} + 2\varepsilon_{s}) + \phi(\varepsilon_{Me} - \varepsilon_{s})\left(\varepsilon_{\parallel}^{0} + 2\right)\right]}{\left(\varepsilon_{\parallel}^{0} + 2\right)(\varepsilon_{Me} + 2\varepsilon_{s}) - \left[(1-\phi)\left(\varepsilon_{\parallel}^{0} - 1\right)(\varepsilon_{Me} + 2\varepsilon_{s}) + \phi(\varepsilon_{Me} - \varepsilon_{s})\left(\varepsilon_{\parallel}^{0} + 2\right)\right]}$$

$$\varepsilon_{\perp} = \frac{(\varepsilon_{\perp}^{0} + 2)(\varepsilon_{Me} + 2\varepsilon_{s}) + 2[(1-\phi)(\varepsilon_{\perp}^{0} - 1)(\varepsilon_{Me} + 2\varepsilon_{s}) + \phi(\varepsilon_{Me} - \varepsilon_{s})(\varepsilon_{\perp}^{0} + 2)]}{(\varepsilon_{\perp}^{0} + 2)(\varepsilon_{Me} + 2\varepsilon_{s}) - [(1-\phi)(\varepsilon_{\perp}^{0} - 1)(\varepsilon_{Me} + 2\varepsilon_{s}) + \phi(\varepsilon_{Me} - \varepsilon_{s})(\varepsilon_{\perp}^{0} + 2)]}$$

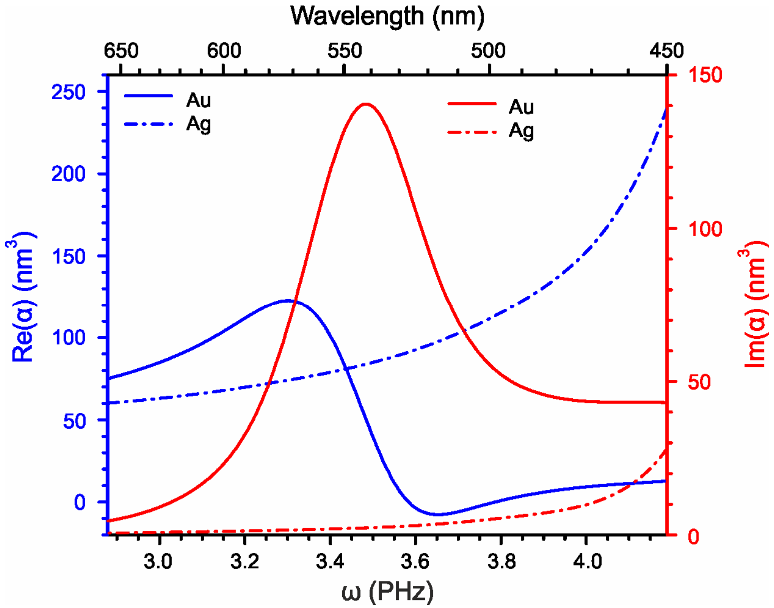
For small NP volume fraction ϕ

$$\varepsilon_{\parallel} \approx \varepsilon_{\parallel}^{0} - \frac{1}{3}\phi\left(\varepsilon_{\parallel}^{0} + 2\right)\left[\varepsilon_{\parallel}^{0} - 1 - \alpha_{s}\left(\varepsilon_{\parallel}^{0} + 2\right)\right]$$

$$\varepsilon_{\perp} \approx \varepsilon_{\perp}^{0} - \frac{1}{3}\phi(\varepsilon_{\perp}^{0} + 2)[\varepsilon_{\perp}^{0} - 1 - \alpha_{s}(\varepsilon_{\perp}^{0} + 2)]$$

$$\alpha_{s} = \varepsilon_{s}\frac{\varepsilon_{Me} - \varepsilon_{s}}{\varepsilon_{Me} + 2\varepsilon_{s}}$$

The real and imaginary parts of the effective polarizability of gold and silver NPs (AuNPs and AgNPs) in the nematic host *5CB*



Frequency dependence of the effective polarizability of AuNP and AgNP of the radius 2.5 nm in the nematic host 4-cyano-4'-pentylbiphenyl (*5CB*)

Shifting of the plasmon resonance frequency in the nematic matrix

Plasmon resonance frequencies

$$\omega_{r\parallel} = \omega_{r0}\left(1 - \phi\varepsilon_s \frac{\varepsilon_\parallel + 2}{2 + 4\varepsilon_s}\right)$$

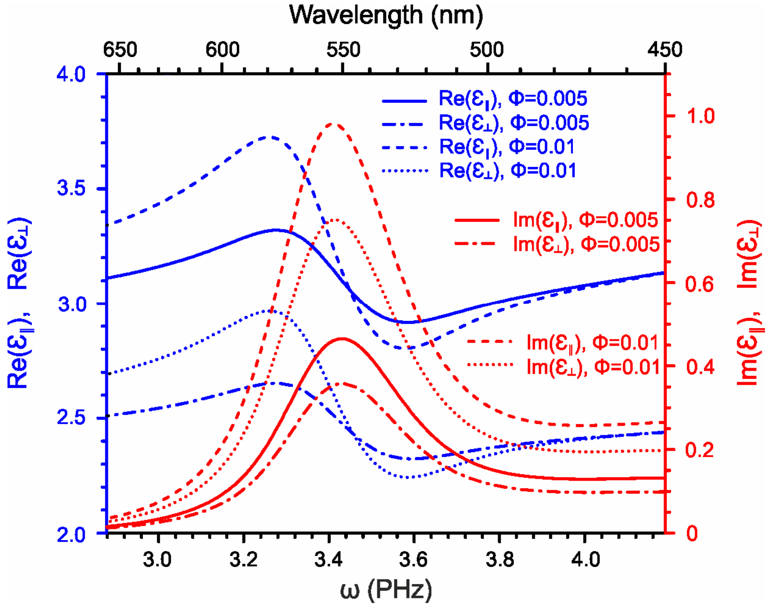
$$\omega_{r\perp} = \omega_{r0}\left(1 - \phi\varepsilon_s \frac{\varepsilon_\perp + 2}{2 + 4\varepsilon_s}\right)$$

The split of the plasmon resonance increases linearly as a function of the NP volume fraction ϕ

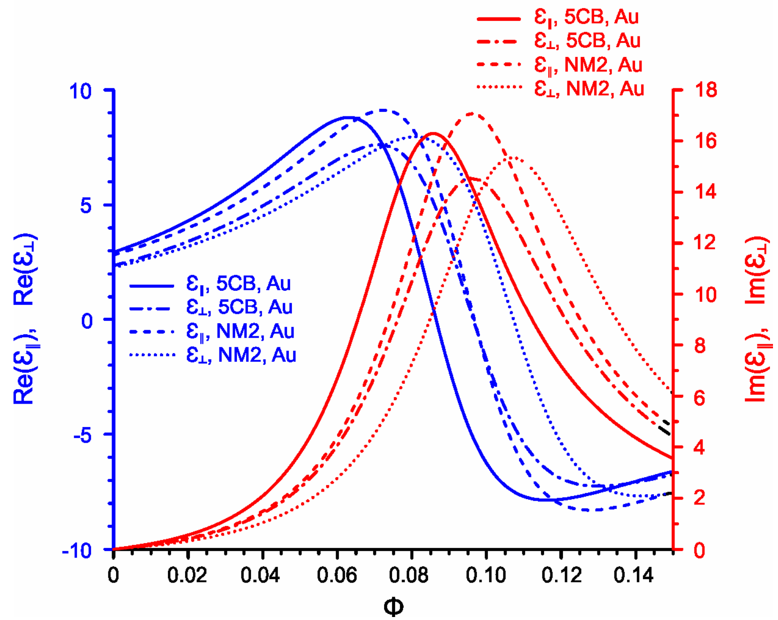
$$\Delta\omega_r = \omega_{r\parallel} - \omega_{r\perp} = -\phi\omega_{r0}\frac{\Delta\varepsilon\varepsilon_s}{2 + 4\varepsilon_s}$$

$$\Delta\varepsilon = \varepsilon_\parallel - \varepsilon_\perp$$

Frequency dependence of the components of the dielectric susceptibility



Frequency dependence of $e(\varepsilon_{\parallel})$ $Im(\varepsilon_{\parallel})$, $Re(\varepsilon_{\perp})$ and $Im(\varepsilon_{\perp})$ of the nematic nanocomposite (host *5CB* plus AuNPs) for the two values of the NP volume fraction $\phi = 0.005$ and $\phi = 0.025$



The dependence of $e(\varepsilon_{\parallel})$ $Im(\varepsilon_{\parallel})$, $Re(\varepsilon_{\perp})$ and $Im(\varepsilon_{\perp})$ on the volume fraction of AuNPs ϕ for the two different nematic hosts *5CB* and *NM2* a fixed wavelength of light $\lambda = 589\ nm$

Liquid crystal NM2 mixture composition:
4-pentyl-4’-cyanobiphenyl 32 wt.%, 4-propyloxy-4’-cyanobiphenyl, 25 wt.%, 4’-cyano-4-biphenyl ester of trans-4-butylcyclohexane-carboxylic acid 20 wt.%, 4-pentyloxy-4’-cyanobiphenyl 13 wt.%, 4-ethoxyphenylester of trans-4-butylcyclohexanecarboxylic acid 10 wt.%

Conclusions

- A molecular-statistical theory of the high frequency dielectric susceptibility of the nematic nano-composites has been developed and approximate analytical expressions for the susceptibility have been obtained in terms of the effective polarizability of NP in the nematic host, volume fraction of NPs and the susceptibility of the pure nematic phase.

- A simple expression for the split of the plasmon resonance of the nanoparticles in the nematic host has been obtained and it has been shown that in the resonance frequency range the high frequency dielectric anisotropy of the nanocomposite may be significantly larger then that of the pure nematic host.

- All dielectric and optical properties of the nanocomposite related to the anisotropy are significantly enhanced which may be important for emerging applications.

- The components of the dielectric susceptibility have been calculated numerically for particular nematic nanocomposites with gold and silver NPs as functions of the nanoparticle volume fraction and frequency.

- The splitting of the plasmon resonance has been observed together with the significant dependence on NP volume fraction and the parameters of the nematic host phase.

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