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GREEN TENSOR IN MATERIAL SCIENCES

44.1 INTRODUCTION

Studies in magneto-optical activity of absorbing nanostructures containing noble metals demand adequate description of radiative corrections that modify the polarizability tensor. The effective medium approximation (EMA) of relative permittivity provides efficient optical properties of composite material thereby the role of nano-elements geometry is unavoidable. The size and/or shape of the particles may be explicitly incorporated within homogenization procedure via depolarization tensor. The so called "strong-couple-dipole" (SCD) method [2] enables to solve this problem explicitly. If the nanoparticles are not vanishingly small, then the spatial extent of associated Green tensor should not be neglected [1]. While the results valid for spherical inclusions are relatively known [3, 4], the other shape variants were so far not be referred in detail. In presented work we develop this method for cylindrical metallic nanoparticles, for which the extended form of depolarization tensor is derived.

The article is organized as follows. The generalized Maxwell-Garnett model of EMA is introduced in the next section. In Sect. 3 the basic principles of the SCD polarizability model are summarized and applied to cylindrical nanoparticles. Numerical results are discussed in the concluding section.

44.2 EFFECTIVE MEDIUM APPROXIMATION

Consider a medium containing volume fraction f of anisotropic metallic nanoparticles randomly distributed in an anisotropic dielectric host. The particles of the same size and shape (not necessarily spheres) are identically oriented; the characteristic dimension of them is supposed to be very small in comparison with wavelength λ of incident electromagnetic field.

If the electrostatic interaction between the nanoparticles is not negligible, it can be taken into account by several ways. In our model, we use the generalized Maxwell-

Garnett approach that enables to consider anisotropic materials; and, also non-spherical particles correspondingly to the above assumptions. It estimates the macroscopic response of the composite as average effect of the dipole field induced in the host medium by different inclusions. This can be done by the Bragg-Pippard model [5] of EMA with the modification for bi-anisotropic case [6,7], in which the effective relative permittivity tensor of composite $\widehat{\varepsilon}_{ef}$ can be written in the form

$$\widehat{\varepsilon}_{ef} = \widehat{\varepsilon}_h + f(\widehat{\varepsilon}_p - \widehat{\varepsilon}_h)\left[f\mathbf{I} + (1-f)\widehat{\boldsymbol{\alpha}}^{-1}(\widehat{\varepsilon}_p - \widehat{\varepsilon}_h)\right]^{-1} , \qquad (44.1)$$

where $\widehat{\varepsilon}_p, \widehat{\varepsilon}_h$ denote the relative permittivity tensors of particles and host medium, respectively. Further, we write $\mathbf{I}$ for the identity matrix and $\widehat{\boldsymbol{\alpha}}$ for the volume averaged polarizability tensor of metallic inclusions.

The polarizability tensor is of great importance to obtain adequate theoretical model of particle polarization properties because of strong dependence on the geometry of particles. In cases when the inclusions are e.g. ellipsoids aligned with principal axes, the polarizability tensor can be expressed in the form

$$\widehat{\boldsymbol{\alpha}} = (\widehat{\varepsilon}_p - \widehat{\varepsilon}_h)\left[\widehat{\varepsilon}_h + \widehat{\mathbf{L}}(\widehat{\varepsilon}_p - \widehat{\varepsilon}_h)\right]^{-1}\widehat{\varepsilon}_h , \qquad (44.2)$$

where $\widehat{\mathbf{L}}$ is diagonal depolarization tensor – see [6] and the references therein. The tensor $\widehat{\mathbf{L}}$ is symmetrical and real-valued; for appropriate orientation of principal axes, it becomes diagonal. Moreover, $\mathrm{Tr}(\widehat{\mathbf{L}}) = 1$ thereby the third diagonal element of $\widehat{\mathbf{L}}$ is coupled with the other two:

$$\widehat{\mathbf{L}} = diag(L_1, L_2, 1 - L_1 - L_2) . \qquad (44.3)$$

The non-zero elements are referred as depolarizing factors.

44.3 SCD POLARIZABILITY

44.3.1 Green tensor

Assuming that the polarization within the particle is uniform, the radiative corrections can be included into polarizability tensor. From general view this problem has been analyzed by Lakhtakia [3], however, with practical consequence only for spherical particles. Nevertheless, the basic principle described there offers possibility to derive polarizability tensor in the other cases by the SCD method.

Without loss of generality, we suppose an isotropic homogeneous host medium, for which $\widehat{\varepsilon}_h = \varepsilon_h\mathbf{I}$. Let us consider a particle of the volume V located at the point $\boldsymbol{x}_0$. Supposing that the electric field inside the particle is constant in the small particle limit together the permittivity tensor $\widehat{\varepsilon}$. The incoming field $\boldsymbol{E}_0$ of the wavelength λ, i.e. with free space wavenumber $k_0 = 2\pi/\lambda$ invokes inside the particle the field of the intensity $\boldsymbol{E}_{ins}$. The corresponding solution of wave equation for the electrical intensity in an anisotropic

media can be written of the form

$$\boldsymbol{E}_{ins} = \boldsymbol{E}_0(\boldsymbol{x}_0) + k_0(\widehat{\boldsymbol{\varepsilon}} - \varepsilon_h \mathbf{I}) \int_V \widehat{\mathbf{G}}(\boldsymbol{x}_0, \boldsymbol{x}) \, dV \, \boldsymbol{E}_{ins} \ . \tag{44.4}$$

The generalized Green function (Green electromagnetic tensor) $\widehat{\mathbf{G}}$ is introduced as the solution of the equation

$$\nabla \times \nabla \times \widehat{\mathbf{G}} - k_0^2 \varepsilon_h \widehat{\mathbf{G}} = \delta(\boldsymbol{x}_0 - \boldsymbol{x}) \mathbf{I} \ , \tag{44.5}$$

where δ stays for the Dirac distribution. The Green tensor can be written as

$$\widehat{\mathbf{G}}(\boldsymbol{x}_0, \boldsymbol{x}) = \left(\mathbf{I} + \frac{1}{k^2} \nabla \otimes \nabla \right) g(\boldsymbol{x}_0, \boldsymbol{x}) \ , \qquad g(\boldsymbol{x}_0, \boldsymbol{x}) = \frac{1}{4\pi} \frac{\mathrm{e}^{ik\|\boldsymbol{x}-\boldsymbol{x}_0\|}}{\|\boldsymbol{x} - \boldsymbol{x}_0\|} \ . \tag{44.6}$$

Here, $k = k_0\sqrt{\varepsilon_h}$; and, g denotes the free space Green function of Helmholtz operator $\Delta + k^2$.

Introducing the average $\langle \widehat{\mathbf{G}} \rangle$ of the Green tensor over the particle volume as

$$|V|\langle \widehat{\mathbf{G}} \rangle = |V| \frac{1}{|V|} \int_V \widehat{\mathbf{G}}(\boldsymbol{x}_0, \boldsymbol{x}') \, dV \ , \tag{44.7}$$

the relation between the fields $\boldsymbol{E}_{ins}$ and $\boldsymbol{E}_0(\boldsymbol{x}_0)$ follows from (44.4) as

$$\boldsymbol{E}_{ins} = \left[\mathbf{I} - |V|\langle \widehat{\mathbf{G}} \rangle (\widehat{\boldsymbol{\varepsilon}} - \varepsilon_h \mathbf{I}) \right]^{-1} \boldsymbol{E}_0(\boldsymbol{x}_0) \ . \tag{44.8}$$

Multiplying the both sides by $\boldsymbol{\varepsilon} - \varepsilon_h \mathbf{I}$ from left, we obtain the equality of induced dipole moments

$$(\boldsymbol{\varepsilon} - \varepsilon_h \mathbf{I}) \boldsymbol{E}_{ins} = (\boldsymbol{\varepsilon} - \varepsilon_h \mathbf{I}) \left[\mathbf{I} - |V|\langle \widehat{\mathbf{G}} \rangle (\widehat{\boldsymbol{\varepsilon}} - \varepsilon_h \mathbf{I}) \right]^{-1} \boldsymbol{E}_0(\boldsymbol{x}_0) \ ,$$

where the right-hand term represents the SCD-generalized polarizability tensor

$$\langle \widehat{\alpha} \rangle = (\boldsymbol{\varepsilon} - \varepsilon_h \mathbf{I}) \left[\mathbf{I} - |V|\langle \widehat{\mathbf{G}} \rangle (\widehat{\boldsymbol{\varepsilon}} - \varepsilon_h \mathbf{I}) \right]^{-1} \ . \tag{44.9}$$

In the described model the particle volume is considered arbitrary small, but not negligible. The volume integral in (44.7) over the volume V with the unit outward normal vector $\boldsymbol{n}$ of its surface S can be rearranged into the form [3]

$$|V|\langle \widehat{\mathbf{G}} \rangle = \int_V \left(\widehat{\mathbf{G}} - \widehat{\mathbf{G}}_s \right) dV - \frac{1}{4\pi k^2} \int_S \frac{\boldsymbol{n} \otimes (\boldsymbol{x} - \boldsymbol{x}_0)}{\|\boldsymbol{x} - \boldsymbol{x}_0\|^3} \, dS \tag{44.10}$$

with the correction term

$$\widehat{\mathbf{G}}_s = \frac{1}{4\pi k^2} \nabla \otimes \nabla \left(\frac{1}{\|\boldsymbol{x} - \boldsymbol{x}_0\|} \right) \ . \tag{44.11}$$

Usually, the surface integral

$$\widehat{\mathbf{L}} = \frac{1}{4\pi} \int_S \frac{\boldsymbol{n} \otimes (\boldsymbol{x} - \boldsymbol{x}_0)}{\|\boldsymbol{x} - \boldsymbol{x}_0\|^3} \, dS \qquad (44.12)$$

predominates in (44.10), therefore, we meet only this one in numerous practical applications. It does not depend on the volume, but only on geometrical shape of the domain V. The singularity at $\boldsymbol{x} = \boldsymbol{x}_0$ can be eliminated by suitably chosen transformation of co-ordinates; possibly, the integration in the sense of Cauchy principal value should be applied.

44.3.2 Cylindrical nanoparticles

We will analyze polarization properties of cylindrical metallic nanoparticle with diameter $d = 2R$ and the height $h = 2H$ in the case, when the cylinder axis is aligned with the incident electromagnetic field $\boldsymbol{E}_0$. The basic form of depolarizing factors derived by (44.12) take the form [4]

$$L_1 = L_2 = \frac{1}{2} \frac{a}{\sqrt{1+a^2}} \ , \qquad L_3 = 1 - \frac{a}{\sqrt{1+a^2}} \ , \qquad (44.13)$$

where $a = h/d$ is the height to diameter ratio.

We focus our attention to the volume integral in (44.10) considering the upper half-cylinder in the co-ordinate system by the Fig. 44.1. Placing the origin into $\boldsymbol{x}_0$ without
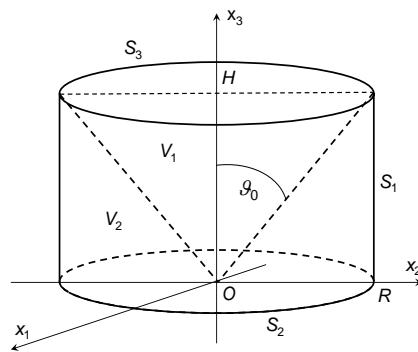

Fig. 44.1 The upper half of cylindrical nanoparticle.

loss of generality and setting $r = \|\boldsymbol{x}\|$, $\boldsymbol{x} = (x_1, x_2, x_3)$, the results of tensor operations in (44.6) and (44.11) can be written as

$$G_{ij} = \frac{e^{ikr}}{4\pi k^2 r^3} \left[\frac{1}{r^2} x_i x_j (3 - 3ikr - k^2 r^2) - \delta_{ij}(1 - ikr - k^2 r^2) \right] \ , \qquad (44.14)$$

$$G_{s,ij} = \frac{1}{4\pi k^2 r^3} \left[\frac{3}{r^2} x_i x_j - \delta_{ij} \right] \ . \qquad (44.15)$$

We divide the half-cylinder by the cone surface $a^2(x_1^2 + x_2^2) = x_3^2$, $0 \le x_3 \le H$, $a = H/R = h/d$ in two sub-regions V_1 and V_2 (see Fig. 44.1), for which we apply spherical

co-ordinates $x_1 = r \cos\varphi \sin\theta$, $x_2 = r \sin\varphi \sin\theta$, $x_3 = r \cos\theta$ with following integration bounds on introduced regions:

$$
\begin{aligned}
V_1 &= \{0 \le \varphi \le 2\pi,\ 0 \le \theta \le \vartheta_0,\ 0 \le r \le H/\cos\theta\}\ , \\
V_2 &= \{0 \le \varphi \le 2\pi,\ \vartheta_0 \le \theta \le \pi/2,\ 0 \le r \le R/\sin\theta\}\ .
\end{aligned}
\tag{44.16}
$$

The integration by the variable φ brings an estimate that the off-diagonal elements are equal to zero, therefore, further we work only with the vectors of diagonal ones that we obtain correspondingly to (44.14), (44.15) in the form

$$
\boldsymbol{z}(r,\theta) = \frac{\mathrm{e}^{\mathrm{i}kr}}{4k^2 r}\left[(1 - \mathrm{i}kr - k^2 r^2)w(\theta)(1,1,-2) + 2k^2 r^2(\sin^3\theta, \sin^3\theta, 2\cos^2\theta\sin\theta)\right]\ ,
\tag{44.17}
$$

$$
\boldsymbol{z}_s(r,\theta) = \frac{1}{4k^2 r}w(\theta)(1,1,-2)\ , \quad w(\theta) = (1 - 3\cos^2\theta)\sin\theta\ .
\tag{44.18}
$$

Thus, the subtraction of above expressions gives

$$
\boldsymbol{z} - \boldsymbol{z}_s = \frac{1}{4k^2}\left[B(r)w(\theta)(1,1,-2) + 2k^2 r^2(\sin^3\theta, \sin^3\theta, 2\cos^2\theta\sin\theta)\right]\ .
\tag{44.19}
$$

The singularity $r = 0$ in the function

$$
B(r) = (\mathrm{e}^{\mathrm{i}kr} - 1)/r - \mathrm{e}^{\mathrm{i}kr}(\mathrm{i}k + k^2 r)
\tag{44.20}
$$

vanishes once the ratio $(\mathrm{e}^{\mathrm{i}kr} - 1)/r$ is expanded into Laurent series with respect to r as

$$
(\mathrm{e}^{\mathrm{i}kr} - 1)/r = \mathrm{i}k - k^2 r - \mathrm{i}k^3 r^2 + \cdots\ .
$$

In the resulting expressions obtained by succeeding integration by the variable r in the bounds from 0 to b the product $kb \ll 1$ on the both sub-regions V_1 and V_2 regarding the assumption $h, d \ll \lambda$. For this reason, the terms with third and higher power of kb are omitted in what follows. After necessary arrangement we obtain

$$
\boldsymbol{y} = \int_0^b (\boldsymbol{z} - \boldsymbol{z}_s)dr = \frac{1}{8}b^2\left[(1 + \cos^2\theta)\sin\theta,\ (1 + \cos^2\theta)\sin\theta,\ 2\cos^2\theta\sin\theta\right]\ .
\tag{44.21}
$$

The bounds of the angle θ are different on V_1 and V_2, moreover, nor b is the same. It means, that the last integration by the variable θ must be splitted. In the region V_1 with $b = H/\cos\theta$ it yields

$$
\int_0^{\vartheta_0} y_1^{(1)}\, d\theta = \frac{1}{8}H^2\frac{\sin^2\vartheta_0}{\cos\vartheta_0}\ , \quad \int_0^{\vartheta_0} y_3^{(1)}\, d\theta = \frac{1}{4}H^2\frac{(1 - \cos\vartheta_0)^2}{\cos\vartheta_0}\ .
\tag{44.22}
$$

At the volume V_2 we have $b = R/\sin\theta$, so that

$$
\int_0^{\vartheta_0} y_1^{(2)}\, d\theta = -\frac{1}{8}R^2\left[\ln\frac{1 - \cos\vartheta_0}{1 + \cos\vartheta_0} + \cos\vartheta_0\right]\ , \quad \int_0^{\vartheta_0} y_3^{(2)}\, d\theta = \frac{1}{4}R^2\cos\vartheta_0\ .
\tag{44.23}
$$

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The summation of above results gives non-zero components of the tensor $\widehat{\mathbf{M}}$; in addition, we must multiply by two because of $V = 2(V_1 \cup V_2)$. To accomplish this derivation, there the substitution $\cos \vartheta_0$ by $a/\sqrt{1 + a^2}$ (see Fig. 44.1) is advantageous to acquire the final relations

$$M_1 = M_2 = -\frac{1}{2}R^2 \ln(\sqrt{1 + a^2} - a), \quad M_3 = R^2 a(\sqrt{1 + a^2} - a). \tag{44.24}$$

The resulting construction of averaged Green tensor (44.10) yields

$$|V|\langle \widehat{\mathbf{G}} \rangle = -\frac{1}{k^2}\left[\widehat{\mathbf{L}} - k^2\widehat{\mathbf{M}}\right] = -\frac{1}{k^2}\widehat{\mathbf{N}}, \tag{44.25}$$

where the elements of $\widehat{\mathbf{M}}$ are given by (44.24); and, we use the depolarizing factors (44.13) in the tensor $\widehat{\mathbf{L}}$. Thus, the polarizability tensor with SCD modification results as

$$\langle \widehat{\boldsymbol{\alpha}} \rangle = (\widehat{\boldsymbol{\varepsilon}} - \varepsilon_h \mathbf{I})\left[\mathbf{I} + \varepsilon_h^{-1}\widehat{\mathbf{N}}(\widehat{\varepsilon}_p - \varepsilon_h \mathbf{I})\right]^{-1}, \tag{44.26}$$

where $\varepsilon_h^{-1} = (k_0/k)^2$. Finally, the elements of $\widehat{\mathbf{N}} = \widehat{\mathbf{L}} - k^2\widehat{\mathbf{M}}$ follow easy as

$$N_1 = N_2 = \frac{1}{2}\frac{a}{\sqrt{1 + a^2}} - \frac{1}{2}k^2 R^2 \ln(\sqrt{1 + a^2} - a), \tag{44.27}$$

$$N_3 = 1 - \frac{a}{\sqrt{1 + a^2}} + k^2 R^2(\sqrt{1 + a^2} - a). \tag{44.28}$$

44.3.3 Numerical results

The elements of basic depolarization tensor $\widehat{\mathbf{L}}$ depend only on the ratio $a = h/d$. The values of the factor L_1 summarized in the Tab. 44.1 increase between 0 and 1 with growing parameter a. With regard to (44.3), the factor L_3 increases.

Tab. 44.1 Depolarization factors L_1 as the function of the ratio $a = h/d$ by (44.13)

L_1		d [nm]				
		2	5	10	20	50
	2	0.3536	0.1857	0.0981	0.0498	0.0200
h	5	0.4642	0.3536	0.2236	0.1213	0.0498
[nm]	10	0.4903	0.4472	0.3536	0.2236	0.0981
	20	0.4975	0.4851	0.4472	0.3536	0.1857
	50	0.4996	0.4975	0.4903	0.4642	0.3536

A similar trend is observed for the correction tensor $k^2\widehat{\mathbf{M}}$, where the influence of the radius R is emphasized. In addition to the tensor $\widehat{\mathbf{L}}$, the values depend also on the incident field wavelength λ as well as on the permittivity of host medium ε_h due the wavenumber k. The data of $k^2 M_1$ in the Tab. 44.2 were calculated correspondingly to the air as the host medium ($\varepsilon_h = 1$) at the wavelength $\lambda = 633$ nm.

Tab. 44.2 Correction term $k^2 M_1$ as the function of the ratio $a = h/d$ by (44.24)

$k^2 M_1$		d [nm]				
		2	5	10	20	50
	2	0.0000	0.0000	0.0000	0.0000	0.0000
h	5	0.0005	0.0003	0.0001	0.0001	0.0000
[nm]	10	0.0028	0.0018	0.0011	0.0006	0.0002
	20	0.0148	0.0103	0.0071	0.0043	0.0019
	50	0.1205	0.0923	0.0712	0.0507	0.0271

CONCLUSIONS

Obtained results offer adequate description of magnetically induced anisotropy in heterogeneous nanostructure with noble metal inclusions for the future application to the magneto-plasmonic sensor element design with the use in biology or chemistry.

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GREEN TENSOR IN MATERIAL SCIENCES

Abstract: *Material properties of heterogeneous nanomaterials modelled by effective medium approximation (EMA) demand specific approaches when metallic inclusions in a host medium are exposed to external magnetic field. Resulting induced anisotropy of permittivity is manifested itself by a specific form of polarizability tensor. In presented work, this one is applied in the so called "strong-couple-dipole" (SCD) method, where the electromagnetic Green tensor is of key importance. The results are oriented to the magneto-plasmonic sensor element design for the use in biology or chemistry.*

Keywords: *anisotropy, effective medium, polarizability tensor, Green tensor.*

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Abstrakt: *Modelování materiálových vlastnosti heterogenních nanomateriálů metodou aproximace efektivním prostředím (EMA) vyžaduje specifický přístup, jsou-li kovové částice v obklopujícím prostředí vystaveny magnetickému poli. Výsledná indukovaná anizotropie permitivity se projevuje specifickou formou tenzoru polarizovatelnosti. Ten je v této práci aplikován prostřednictvím tzv. metody silně vázaných dipólů (SCD), kde se klíčovým způsobem uplatňuje Greenův (elektromagnetický) tenzor. Výsledky směřují k návrhu magneto-plasmonického senzoru s užitím v bilogii a chemii.*

Klíčová slova: *anizotropie, efektivní prostředí, tenzor polarizovatelnosti, Greenův tenzor.*

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