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Single-layer model of reflective nanostructures for magneto-ellipsometry data analysis

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Abstract. In this work we present the method of magneto-ellipsometry data analysis. Magneto-ellipsometry measurements are conducted in situ during nanostructures synthesis. Magnetic field is applied in configuration of magneto-optical transverse Kerr effect. Single-layer model of reflective nanostructures is in focus.

1. Introduction

Magneto-ellipsometry is considered as one of powerful reliable nondestructive methods for nanostructures synthesis control that is highly important for spintronics, electronics and nanotechnology. This technique combines ellipsometry and magneto-optical Kerr effect measurements. Magneto-ellipsometry has to be developed and in this work we report on magneto-ellipsometry measurements analysis for the case of single-layer nanostructures study. We have developed the approach that can be applied to investigation of reflective ferromagnetic/non-ferromagnetic nanostructures that are a subject of interest due to observed spin transport phenomena. We offer an algorithm that yields information about dielectric permittivity tensor of ferromagnetic layer [1], where diagonal tensor elements are responsible for refractive index and extinction coefficient, off-diagonal tensor elements are related to magneto-optical effects:

$$[\varepsilon]=\begin{bmatrix}\varepsilon_{11} & \varepsilon_{12} & 0\\ \varepsilon_{21} & \varepsilon_{22} & 0\\ 0 & 0 & \varepsilon_{33}\end{bmatrix}=\begin{bmatrix}\varepsilon'_{11}-i\varepsilon''_{11} & -i(\varepsilon'_{12}-i\varepsilon''_{12})(Q_1-iQ_2) & 0\\ i(\varepsilon'_{12}-i\varepsilon''_{12})(Q_1-iQ_2) & \varepsilon'_{11}-i\varepsilon''_{11} & 0\\ 0 & 0 & \varepsilon'_{11}-i\varepsilon''_{11}\end{bmatrix}, \quad (1)$$

where ε is a complex permittivity of a medium ($\varepsilon_{11}=\varepsilon_{22}\approx\varepsilon_{33}$, $\varepsilon_{12}=-\varepsilon_{21}$), real parts are marked by ', imaginary by ", $Q=Q_1-iQ_2$ is a proportional to magnetization magneto-optical parameter. In the non-magnetic condition ($Q=0$) the off-diagonal tensor elements vanish.

In the following, we describe the method of interpretation of the ellipsometric and magneto-ellipsometric measurements data from the in situ setup of a magneto-optical generalized ellipsometer, which is integrated into an ultra-high vacuum chamber with the electromagnet for magnetization reversal of the sample. The key idea of this approach and the case of the model of a homogeneous semi-infinite medium have been reported in [2] and at the 8th Joint European Magnetic Symposia (JEMS-2016) [3]. Here we repeat some of our basic ideas and present developed expressions for experimental data processing for a single-layer model of reflective nanostructures in order to study their optical and magneto-optical properties. We consider the case of electromagnetic wave incidence from non-magnetic dielectric medium (characterized by the refraction index N_0) onto ferromagnetic metal (the refraction index N_1) on substrate (the refraction index N_2). We set the magnetization vector to be z-axis directed, so that YX plane is a plane of incidence, YZ plane is a boundary plane. The transverse configuration is in focus because of the design features of high-vacuum chamber and electromagnet that are commonly used for magnetization reversal. In this paper, we consider the visible light range, as a great amount of modern ellipsometers work in this range.

2. Ellipsometry and magneto-ellipsometry measurements data

Let us denote the ellipsometric parameters in the non-magnetic condition ($Q=0$) as ψ_0 and Δ_0 [1]. In the case of magneto-ellipsomertic characterization of the sample ($Q=Q_1-iQ_2\neq 0$) the surface transverse magneto-optical Kerr effect results in the ellipsometric angles corrections $\delta\psi$ and $\delta\Delta$. Thus, the ellipsometric parameters become $\psi_0+\delta\psi$, $\Delta_0+\delta\Delta$. It means that four independent real-valued quantities (ψ_0, $\delta\psi$, Δ_0, $\delta\Delta$) are measured and, as a result, four real-valued quantities (ε'_{11}, ε''_{11}, ε'_{12}, ε''_{12}) can be derived.

To start analysis of magneto-ellipsometry experimental data (ψ and Δ) we have to write the real and imaginary parts of complex reflection coefficients in the basic equation of ellipsometry [4, 5]:

$$\rho = tg(\psi_0+\delta\psi)\exp(i(\Delta_0+\delta\Delta)) = R_p R_S^{-1} = (R'_p - iR''_p)(R'_S - iR''_S)^{-1}, \tag{2}$$

where ρ is the complex ellipsometric parameter, R_p and R_s are complex reflection coefficients corresponding to in-plane p-polarization and out-of-plane s-polarization respectively, real parts again are marked by ', imaginary by ". According to mode conversion from the p to the s polarized channel we can write that

$$R_p = R_{pp} + R_{ps} = R'_{p0} + R'_{p1} - i(R''_{p0} + R''_{p1}), \tag{3}$$

$$R_S = R_{SS} + R_{sp} = R_{S0} = R'_{S0} - iR''_{S0}, \tag{4}$$

where we have distinguished the magnetic field contribution and marked it by subscript 1, non-magnetic summands – by subscript 0. One can see that transverse Kerr effect yields to $R''_{s1}=0$, $R'_{s1}=0$.

By substituting equations (3-4) into (2) we obtain for non-magnetic condition:

$$tg\psi_0 = \sqrt{\frac{(R'_{p0}R'_{S0} + R''_{S0}R''_{p0})^2 + (R''_{S0}R'_{p0} - R''_{p0}R'_{S0})^2}{{R'_{S0}}^2 + {R''_{S0}}^2}}, \tag{5}$$

$$\Delta_0 = arctg\frac{R''_{S0}R'_{p0} - R''_{p0}R'_{S0}}{R'_{p0}R'_{S0} + R''_{p0}R''_{S0}}, \tag{6}$$

while the influence of an external magnetic field leads to ellipsometric parameters $\delta\psi$ and $\delta\Delta$:

$$\delta\psi = \psi - \psi_0 = arc\,tg\left(F\,tg(\psi_0)\right) - \psi_0, \tag{7}$$

$$\delta\Delta = \Delta - \Delta_0 = arctg\frac{R''_{S0}(R'_{p0}+R'_{p1}) - (R''_{p0}+R''_{p1})R'_{S0}}{(R'_{p0}+R'_{p1})R'_{S0} + (R''_{p0}+R''_{p1})R''_{S0}} - arctg\frac{R''_{S0}R'_{p0} - R''_{p0}R'_{S0}}{R'_{p0}R'_{S0} + R''_{p0}R''_{S0}}, \tag{8}$$

where F is a helpful notation:

$$tg\left(\psi_0+\delta\psi\right) = F\,tg\left(\psi_0\right) = tg\left(\psi_0\right)\times$$
$$\times\sqrt{1 + \frac{(R''_{S0}R''_{p1})^2 + (R''_{p1}R'_{S0})^2 + 2R''_{p0}R''_{p1}({R'_{S0}}^2 + {R''_{S0}}^2)}{(R'_{p0}R'_{S0} + R''_{p0}R''_{S0})^2 + \left(R''_{S0}R'_{p0} - R''_{p0}R'_{S0}\right)^2} + \frac{(R'_{p1}R'_{S0})^2 + (R'_{p1}R''_{S0})^2 + 2R'_{p0}R'_{p1}({R'_{S0}}^2 + {R''_{S0}}^2)}{(R'_{p0}R'_{S0} + R''_{p0}R''_{S0})^2 + \left(R''_{S0}R'_{p0} - R''_{p0}R'_{S0}\right)^2}}. \tag{9}$$

3. Data analysis

In Figure 1 one can see a diagram of single-layer model, where 0 – ambient medium, 1 – ferromagnetic metal (d – thickness), 2 – substrate, φ_0, φ_1 and φ_2 are the angles of incidence and refraction and related to each other by Snell's law.

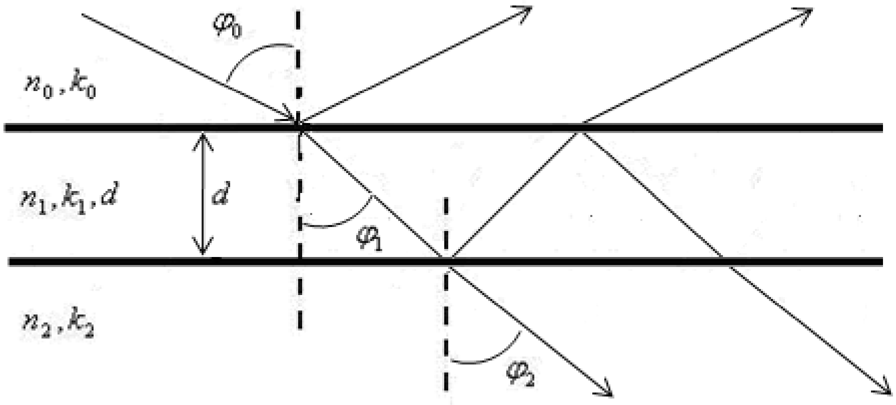

Figure 1. Single-layer model of reflective nanostructures

For a single-layer model complex refractive indices of the material under study ($N_1=n_1-ik_1$) are calculated from ψ_0, Δ_0 measurements by the Nelder-Mead method. The values of $N_0=n_0-ik_0$, $N_1=n_1-ik_1$, $N_2=n_2-ik_2$ are necessary for the following ellipsometric angles calculation.

Analytical expressions for the Fresnel coefficients that take into account the magneto-optical parameter in the off-diagonal permittivity tensor elements were presented in [2, 4]. It was shown that the following expressions should be used for a single-layer model:

$$R_p = r_{01p} + \frac{t_{01p} t_{10p} r_{12p} \exp(-i2\beta)}{1 - r_{10p} r_{12p} \exp(-i2\beta)}, \tag{10}$$

$$R_S = \frac{r_{01S} + r_{12S} \exp(-i2\beta)}{1 + r_{01S} r_{12S} \exp(-i2\beta)}, \tag{11}$$

$$r_{01p} = \frac{N_1 \cos\varphi_0 - N_0 \cos\varphi_1}{N_1 \cos\varphi_0 + N_0 \cos\varphi_1} - i \frac{2QN^2{}_0 \sin\varphi_0 \cos\varphi_0}{(N_1 \cos\varphi_0 + N_0 \cos\varphi_1)^2}, \tag{12}$$

$$r_{12p} = \frac{N_2 \cos\varphi_1 - N_1 \cos\varphi_2}{N_2 \cos\varphi_1 + N_1 \cos\varphi_2} - i \frac{2QN^2{}_1 \sin\varphi_1 \cos\varphi_1}{(N_2 \cos\varphi_1 + N_1 \cos\varphi_2)^2}, \tag{13}$$

$$r_{10p} = \frac{N_0 \cos\varphi_1 - N_1 \cos\varphi_0}{N_0 \cos\varphi_1 + N_1 \cos\varphi_0} + i \frac{2QN^2{}_1 \sin\varphi_1 \cos\varphi_1}{(N_0 \cos\varphi_1 + N_1 \cos\varphi_0)^2}, \tag{14}$$

$$r_{01S} = \frac{N_0 \cos\varphi_0 - N_1 \cos\varphi_1}{N_0 \cos\varphi_0 + N_1 \cos\varphi_1}, \tag{15}$$

$$r_{12S} = \frac{N_1 \cos\varphi_1 - N_2 \cos\varphi_2}{N_1 \cos\varphi_1 + N_2 \cos\varphi_2}, \tag{16}$$

$$t_{01p} = \frac{2N_0 \cos\varphi_0}{N_1 \cos\varphi_0 + N_0 \cos\varphi_1} + i \frac{2QN^3{}_0 \sin\varphi_0 \cos\varphi_0}{N_1 (N_1 \cos\varphi_0 + N_0 \cos\varphi_1)^2}, \tag{17}$$

$$t_{10p} = \frac{2N_1 \cos\varphi_1}{N_1 \cos\varphi_0 + N_0 \cos\varphi_1} - i \frac{2QN^3{}_1 \sin\varphi_1 \cos\varphi_1}{N_0 (N_1 \cos\varphi_0 + N_0 \cos\varphi_1)^2}, \tag{18}$$

$$\beta_1 = \frac{2\pi}{\lambda} N_1 \cos\varphi_1 d_1, \tag{19}$$

where β_1 is phase thickness of the film. Indices r_{01p}, r_{01s} and r_{12p}, r_{12s} in expressions (12, 15) and (13, 16) are the refractive indices for interfaces 0-1 and 1-2, respectively. Indices t_{01p} and t_{10p} in expressions (17, 18) are transmission coefficients. Indices r_{01p} and t_{01p} correspond to the wave propagation from medium 0 to medium 1, while r_{10p} and t_{10p} – to the backward propagation. Taking into account expressions (3, 4) let us write r_{01p}, r_{12p}, r_{01s}, r_{12s}, r_{10p}, t_{01p}, t_{10p} in the same manner as the refractive indices and transmission coefficients for the model of a homogeneous semi-infinite medium:

$$r_{01S} = (R'_{S0})_{01} - i(R''_{S0})_{01}. \tag{20}$$

$$r_{12S} = (R'_{S0})_{12} - i(R''_{S0})_{12}. \tag{21}$$

$$r_{01p} = (R'_{p0})_{01} + (R'_{p1})_{01} - i((R''_{p0})_{01} + (R''_{p1})_{01}) = rr_{01} - i\ ri_{01}, \tag{22}$$

$$r_{12p} = (R'_{p0})_{12} + (R'_{p1})_{12} - i((R''_{p0})_{12} + (R''_{p1})_{12}) = rr_{12} - i\ ri_{12}, \tag{23}$$

$$r_{10p} = (R'_{p0})_{10} + (R'_{p1})_{10} - i((R''_{p0})_{10} + (R''_{p1})_{10}) = rr_{10} - i\ ri_{10}, \tag{24}$$

$$t_{01p} = (T'_{p0})_{01} + (T'_{p1})_{01} - i((T''_{p0})_{01} + (T''_{p1})_{01}) = tr_{01} - i\ ti_{01}, \tag{25}$$

$$t_{10p} = (T'_{p0})_{10} + (T'_{p1})_{10} - i((T''_{p0})_{10} + (T''_{p1})_{10}) = tr_{10} - i\ ti_{10}, \tag{26}$$

where $(R'_{s0})_{01}$, $(R''_{s0})_{01}$, $(R'_{p0})_{01}$, $(R''_{p0})_{01}$, $(R'_{p1})_{01}$, $(R''_{p1})_{01}$ are R'_{s0}, R''_{s0}, R'_{p0}, R''_{p0}, R'_{p1}, R''_{p1} in the model of a homogeneous semi-infinite medium, respectively. Subscript 01 denotes the electromagnetic wave incidence from ambient medium 0 onto layer 1. Indices $(R'_{s0})_{12}$, $(R''_{s0})_{12}$, $(R'_{p0})_{12}$, $(R''_{p0})_{12}$, $(R'_{p1})_{12}$, $(R''_{p1})_{12}$ are also calculated by formulae for the model of a homogeneous semi-infinite medium, the only difference is that subscript 12 denotes the electromagnetic wave incidence from layer 1 onto substrate 2 that leads to the following changes: $\cos\varphi_0 \to \cos\varphi_1$, $\cos\varphi_1 \to \cos\varphi_2$, $\sin\varphi_0 \to \sin\varphi_1$, $n_1 \to n_2$, $n_0 \to n_1$, $k_1 \to k_2$, $k_0 \to k_1$. Likewise, indices $(R'_{p0})_{10}$, $(R''_{p0})_{10}$, $(R'_{p1})_{10}$, $(R''_{p1})_{10}$ describe the electromagnetic wave propagation from layer 1 to medium 0: $\cos\varphi_0 \leftrightarrow \cos\varphi_1$, $\sin\varphi_0 \leftrightarrow \sin\varphi_1$, $n_0 \leftrightarrow n_1$, $k_0 \leftrightarrow k_1$.

Transmission coefficients were not involved into algorithm of data processing for the model of a homogeneous semi-infinite medium. Therefore, we report on $(T'_{p0})_{01}$, $(T''_{p0})_{01}$, $(T'_{p1})_{01}$, $(T''_{p1})_{01}$ here:

$$(T'_{p0})_{01} = 2\frac{(n_0 n_1 + k_0 k_1)(a^2 + c^2) + (n_0{}^2 + k_0{}^2)(ab + cd)}{A_3{}^2 + B_3{}^2}, \tag{27}$$

$$(T''_{p0})_{01} = 2\frac{(n_0{}^2 + k_0{}^2)(ad - bc) + (n_1 k_0 - n_0 k_1)(a^2 + c^2)}{A_3{}^2 + B_3{}^2}, \tag{28}$$

$$(T'_{p1})_{01} = 2\frac{Q_1(pq + rs) - Q_2(pr - sq)}{(n_1{}^2 + k_1{}^2)(A_3{}^2 + B_3{}^2)^2}, \tag{29}$$

$$(T''_{p1})_{01} = 2\frac{Q_1(pr - sq) + Q_2(pq + rs)}{(n_1{}^2 + k_1{}^2)(A_3{}^2 + B_3{}^2)^2}, \tag{30}$$

where

$$A_3 = n_1 a + k_1 c + n_0 b + k_0 d, \tag{31}$$

$$B_3 = k_1 a - n_1 c + k_0 b - n_0 d, \tag{32}$$

$$p = N(3n_0^2 k_0 - k_0^3) + P(n_0^3 - 3n_0 k_0^2), \tag{33}$$

$$q = n_1(A_3{}^2 - B_3{}^2) - 2A_3 B_3 k_1, \tag{34}$$

$$r = k_1(B_3{}^2 - A_3{}^2) - 2A_3 B_3 n_1, \tag{35}$$

$$s = N(n_0^3 - 3n_0 k_0^2) - P(3n_0^2 k_0 - k_0^3), \quad (36)$$
$$a = \mathrm{Re}(\cos\varphi_0), \quad (37)$$
$$b = \mathrm{Re}(\cos\varphi_1), \quad (38)$$
$$c = \mathrm{Im}(\cos\varphi_0), \quad (39)$$
$$d = \mathrm{Im}(\cos\varphi_1), \quad (40)$$
$$N = \mathrm{Re}(\sin\varphi_0)a - \mathrm{Im}(\sin\varphi_0)\mathrm{c} \quad (41)$$
$$P = -\mathrm{Re}(\sin\varphi_0)c - \mathrm{Im}(\sin\varphi_0)a \quad (42)$$

Coefficients $(T'_{p0})_{10}$, $(T''_{p0})_{10}$, $(T'_{p1})_{10}$, $(T''_{p1})_{10}$ correspond to the electromagnetic wave propagation from layer 1 to medium 0, that leads to the changes: $\cos\varphi_0 \leftrightarrow \cos\varphi_1$, $\sin\varphi_0 \leftrightarrow \sin\varphi_1$, $n_0 \leftrightarrow n_1$, $k_0 \leftrightarrow k_1$.

Let us take into account $N_0=n_0-ik_0$, $N_1=n_1-ik_1$, $N_2=n_2-ik_2$, $Q=Q_1-iQ_2$ and compare expressions (10, 11) with (2, 3). Thus we obtain expressions for R'_{p0}, R''_{p0}, R'_{p1}, R''_{p1}, R'_{s0} and R''_{s0}.

$$R'_{p0} = (((R'_{p0})_{01} + \xi_1(R'_{p0})_{12} - \eta_1(R''_{p0})_{12})(1+\xi_1 L_{0112} - \eta_1 M_{0112}) +$$
$$+((R''_{p0})_{01} + \eta_1(R'_{p0})_{12} + \xi_1(R''_{p0})_{12})(\xi_1 M_{0112} + \eta_1 L_{0112}))((1+\xi_1 L_{0112} - \eta_1 M_{0112})^2 + (\xi_1 M_{0112} + \eta_1 L_{0112})^2)^{-1}, \quad (43)$$
$$R''_{p0} = (((R''_{p0})_{01} + \eta_1(R'_{p0})_{12} + \xi_1(R''_{p0})_{12})(1+\xi_1 L_{0112} - \eta_1 M_{0112}) -$$
$$-((R'_{p0})_{01} + \xi_1(R'_{p0})_{12} - \eta_1(R''_{p0})_{12})(\xi_1 M_{0112} + \eta_1 L_{0112}))((1+\xi_1 L_{0112} - \eta_1 M_{0112})^2 + (\xi_1 M_{0112} + \eta_1 L_{0112})^2)^{-1}, \quad (44)$$
$$R'_{p1} = \frac{\Omega\chi - \Gamma\varpi}{\Omega^2 + \Gamma^2} - R'_{p0}, \quad (45)$$
$$R''_{p1} = \frac{\Omega\varpi + \Gamma\chi}{\Omega^2 + \Gamma^2} - R''_{p0}, \quad (46)$$
$$R'_{S0} = (((R'_{S0})_{01} + \xi_1(R'_{S0})_{12} - \eta_1(R''_{S0})_{12})(1+\xi_1 H_{0112} - \eta_1 J_{0112}) +$$
$$+((R''_{S0})_{01} + \eta_1(R'_{S0})_{12} + \xi_1(R''_{S0})_{12})(\xi_1 J_{0112} + \eta_1 H_{0112}))((1+\xi_1 H_{0112} - \eta_1 J_{0112})^2 + (\xi_1 J_{0112} + \eta_1 H_{0112})^2)^{-1}, \quad (47)$$
$$R''_{S0} = (((R''_{S0})_{01} + \eta_1(R'_{S0})_{12} + \xi_1(R''_{S0})_{12})(1+\xi_1 H_{0112} - \eta_1 J_{0112}) -$$
$$-((R'_{S0})_{01} + \xi_1(R'_{S0})_{12} - \eta_1(R''_{S0})_{12})(\xi_1 J_{0112} + \eta_1 H_{0112}))((1+\xi_1 H_{0112} - \eta_1 J_{0112})^2 + (\xi_1 J_{0112} + \eta_1 H_{0112})^2)^{-1}, \quad (48)$$

where the following notations are used:

$$L_{0112} = (R'_{p0})_{12}(R'_{p0})_{01} - (R''_{p0})_{12}(R''_{p0})_{01}, \quad (49)$$
$$M_{0112} = (R'_{p0})_{01}(R''_{p0})_{12} + (R'_{p0})_{12}(R''_{p0})_{01}, \quad (50)$$
$$\xi_1 = \mathrm{Re}(\exp(-i2\beta_1)), \quad (51)$$
$$\eta_1 = -\mathrm{Im}(\exp(-i2\beta_1)), \quad (52)$$
$$J_{0112} = (R'_{S0})_{01}(R''_{S0})_{12} + (R'_{S0})_{12}(R''_{S0})_{01}, \quad (53)$$
$$H_{0112} = (R'_{S0})_{01}(R'_{S0})_{12} - (R''_{S0})_{12}(R''_{S0})_{01}, \quad (54)$$
$$\Omega = 1 - \xi_1(rr_{10}rr_{12} - ri_{10}ri_{12}) + \eta_1(ri_{10}rr_{12} + rr_{10}ri_{12}), \quad (55)$$
$$\varpi = ri_{01} - (\xi_1 rr_{12} - \eta_1 ri_{12})(ri_{01}rr_{10} + ri_{10}rr_{01} - \tau) - (\xi_1 ri_{12} + \eta_1 rr_{12})(rr_{01}rr_{10} - ri_{01}ri_{10} - \theta), \quad (56)$$
$$\Gamma = \xi_1(ri_{10}rr_{12} + rr_{10}ri_{12}) + \eta_1(rr_{10}rr_{12} - ri_{10}ri_{12}), \quad (57)$$
$$\chi = rr_{01} - (\xi_1 rr_{12} - \eta_1 ri_{12})(rr_{01}rr_{10} - ri_{01}ri_{10} - \theta) + (\xi_1 ri_{12} + \eta_1 rr_{12})(ri_{01}rr_{10} + ri_{10}rr_{01} - \tau), \quad (58)$$
$$\theta = tr_{01}tr_{10} - ti_{01}ti_{10}, \quad (59)$$
$$\tau = ti_{01}tr_{10} + ti_{10}tr_{01}. \quad (60)$$

Thus, we have all formulae that are necessary for theoretical calculation of the ellipsometric angles (2-9) in case of a single-layer model. Final step is giving the best fit to the experimental data by the use of the wavelength-to-wavelength Nelder–Mead minimization of the ellipsometric angles. It yields the spectral dependences of real (Q_1) and imaginary parts (Q_2) of magneto-optical parameter Q. So, we have information about all elements of the dielectric permittivity tensor.

4. Conclusion

To conclude, we have proposed an approach to studying single-layer nanomaterials by means of magneto-ellipsometry. The algorithm of experimental data analysis (ψ_0, Δ_0, $\psi_0+\delta\psi$, $\Delta_0+\delta\Delta$) is presented. As a result, optical and magneto-optical properties can be easily and reliably characterized during synthesis.

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