Progress In Electromagnetics Research Letters, Vol. 54, 71–77, 2015

Calculation of Optical Waves Propagation through Gyrotropic Anisotropic Media: lr- and sp-Polarization

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Abstract—A new method of electrodynamic analysis of gyrotropic (isotropic and anisotropic) media is developed. This method is based on the scalar representation of Maxwell's equations corresponding to 4×4-matrix formulation and coupling equations for gyrotropic medium in the Drude's form. It is utilized by solving the wave equations of second and fourth order, followed by cross-linking the fields at the boundary. The obtained results are experimentally verified by their good matching with the popular benchmark data, such as quartz rotatory power and in comparison with a known standard parameter of an optical element, such as $\lambda/4$-plate. This method simply summarizes the polarimetric and ellipsometric calculations.

In 1972, Berreman finally formulated a theoretical approach to the electrodynamics of condensed matter [1], first introduced by Teitler and Henvis [2], called 4×4-matrix technique or 4×4-matrix formulation. According to this approach, the Maxwell's equations, along with the constitutive equations (also referred to as coupling equations) for a particular optical media, shall be converted into a scalar system of four first order differential equations in four unknowns, which are the field components E_x, E_y, H_x, H_y in the Cartesian coordinates system. These components should be chosen in the following way. Let us consider a plane wave propagating from vacuum (air) in the xz plane of incidence in the direction of the z axis, perpendicular to the plane xy, which is a boundary of the medium under investigation. The field components along the x axis are assumed to be $\sim \exp(ik_x x)$, where k_x is a coordinate along the axis of the wave vector $\mathbf{k}_0$ of the reflected wave and the wave vector $\mathbf{k}$ of the refracted wave. The y coordinate is expected to be $\partial/\partial y = 0$. This makes it possible to eliminate components E_z and H_z in a scalar system of the six first order differential equations equivalent to the Maxwell's vector equations.

The Berreman's method is a commonly used algebraic method for solving the matrix wave equation. It is reduced to the calculation of the eigenvalue problem for a 4×4-matrix. However, the amount of calculation in the corresponding numerical method is too high, which makes its practical implementation difficult.

Nevertheless, it is difficult to overestimate the importance of the 4×4-matrix representation due to the initial presentation of Maxwell equations as four scalar differential equations. This paper presents a new method for solving this problem. Its main advantage when compared to the Berreman's method is computational efficiency. It is interesting that it is not necessary to use the flow of matrix transformations, but to use only the basic theory of ordinary differential equations. For simplicity, but without loss of generality, we will reduce our considerations here to some extension of the general case of an anisotropic gyrotropic medium, combining two cases discussed in [1], namely orthorhombic crystal and certain optically active medium. We will benefit from an important fact that a 4×4-matrix of scalar equations is a sparse matrix, because more than a half of the coefficients of the system (the matrix elements) are equal to zero. As will be shown below, this makes it possible to substitute a system of

Received 24 March 2015, Accepted 30 June 2015, Scheduled 22 July 2015
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four first order equations by a simpler system of two second-order equations. In the case of a gyrotropic medium the field components E_x and E_y (H_x and H_y) are dependent and coupled. A regular vision of the basis of the two linearly independent waves comes back, if we consider the circular left l-wave and right r-wave.

Let us go ahead and consider the following question. What will be the wave equation of order higher than the second for some components of the field, if we formally consider the s- and p-polarizations, as the basis of independent s- and p-waves no longer exists? It is wonderful that such an equation exists. It is the fourth-order equation for E_y. This means that we can consider the s-wave as independent. This makes it possible to design a simple technique of calculations for finding the reflection and transmission of light at the boundaries of gyrotropic anisotropic plane-parallel plate (film) both at normal and at oblique incidence of the wave. In turn, we are able to combine polarimetric and ellipsometric evaluations in a common scheme [3]. The corresponding results will be illustrated below using simulation examples.

Let us take the Maxwell equations in the Landau and Lifshitz [4] representation where we set $\mathbf{H} \equiv \mathbf{B}$ and where the effects of a small deviation of the magnetic permeability of the units are included in the dielectric tensor

$$\nabla \times \mathbf{H} = \frac{i\omega}{c}\mathbf{D}, \quad \nabla \times \mathbf{E} = -\frac{i\omega}{c}\mathbf{H}. \tag{1}$$

Here, the dependence of the fields $\mathbf{E}$, $\mathbf{H}$ and $\mathbf{D}$ from time t at a frequency ω is built according to the harmonic rule $\sim \exp(i\omega t)$, where c is the speed of light in vacuum.

Let us consider the orthorhombic crystal with a regular optical activity. Its coupling equation for the electric displacement $\mathbf{D}$ and the electric vector $\mathbf{E}$ is

$$\mathbf{D} = \hat{\varepsilon}\mathbf{E} + \gamma\nabla \times \mathbf{E}, \tag{2}$$

where $\hat{\varepsilon}$ is a second rank diagonal complex tensor and γ an optical activity index introduced by Drude [5] associated with the rotatory power (it will be shown below how exactly this association is established). The system (1) with the constitutive Equation (2) is equivalent to the system of six scalar equations. Two of them do not contain the derivatives

$$ik_xH_y = ik_0\varepsilon_{zz}E_z + \gamma k_0^2 H_z, \quad k_xE_y = -k_0H_z, \tag{3}$$

where $k_x = k_0 \sin\phi_0$, $k_0 = \omega/c = 2\pi/\lambda$, ϕ_0 — an angle of incidence, and λ is the wavelength in vacuum.

Solving (3) for E_z and H_z and substituting these values in the remaining four equations that contain derivatives, we obtain a fourth order system with the unknowns E_x, E_y, H_x, H_y, which can be written as follows

$$\begin{cases} E'_x = & m_{12}E_y & & +m_{14}H_y, \\ E'_y = & & m_{23}H_x, & \\ H'_x = & m_{32}E_y & & +m_{34}H_y, \\ H'_y = m_{41}E_x & & +m_{43}H_x, & \end{cases} \tag{4}$$

where

$$m_{12} = \frac{\gamma k_x^2}{\varepsilon_{zz}}, \quad m_{14} = -\frac{ik_z^2}{k_0\varepsilon_{zz}}, \quad m_{23} = ik_0,$$
$$m_{32} = \frac{ik_y^2}{k_0}, \quad m_{34} = k_0^2\gamma, \quad m_{41} = -ik_0\varepsilon_{xx}, \quad m_{43} = -k_0^2\gamma,$$
$$k_y^2 = k_0^2\varepsilon_{yy} - k_x^2, \quad k_z^2 = k_0^2\varepsilon_{zz} - k_x^2.$$

Hereafter, the prime ($'$) denotes differentiation with respect to z. Let us consider the following two cases: i) the transformation to a system of two second order coupled equations and ii) the transformation to a single fourth order equation. Hence we obtain the following.

i) From the first and second equations of (4) we may express H_x and H_y through E_x and E_y and substitute them in the third and fourth equations of this system. As a result, we obtain a system of two second-order equations

$$E''_y + a_1E'_x + b_1E_y = 0, \quad E''_x + a_2E'_y + b_2E_x = 0, \tag{5}$$

where

$$a_1 = \frac{k_0^4 \gamma \varepsilon_{zz}}{k_z^2}, \quad b_1 = k_y^2 - \frac{k_0^4 \gamma^2 k_x^2}{k_z^2}, \quad a_2 = -k_0^2 \gamma, \quad b_2 = \frac{\varepsilon_{xx}}{\varepsilon_{zz}} k_z^2.$$

Similarly, we obtain a system for magnetic components H_x and H_y. The systems for electric and magnetic components are identical, while for isotropic media and at normal incidence they have the following form:

$$\begin{cases} E_y'' + k_0^2 \gamma E_x' + k_0^2 \varepsilon E_y = 0, \\ E_x'' - k_0^2 \gamma E_y' + k_0^2 \varepsilon E_x = 0, \end{cases} \tag{6}$$

where ε is a dielectric constant.

It should be noted that the system of Equation (6) describes free mechanical gyrator, where E_x and E_y represent two general coordinates of the system, and z – the time [6]. Thus, we have a model of the electromagnetic gyrator, whose existence was noticed in Tellegen's remarkable work [6].

Let us now add the first equation from the system (6) to the second one two times, multiplying it first time by the imaginary unit i, and then by $-i$. In this way, we obtain an equation for the left and right circularly polarized waves

$$\Phi_\pm'' \pm i k_0^2 \gamma \Phi_\pm' + k_0^2 \varepsilon \Phi_\pm = 0, \tag{7}$$

where $\Phi_\pm = E_x \pm i E_y$.

Two independent particular solutions of (7) are

$$\Phi_\pm(z) = \exp\left\{ -i k_0 \left(\pm \frac{k_0 \gamma}{2} + \sqrt{\varepsilon + \frac{k_0^2 \gamma^2}{4}} \right) z \right\} \tag{8}$$

They describe the waves of left and right circular polarization. The difference in the refractive indices for distinct circular polarization is

$$|n_+ - n_-| = k_0 \gamma. \tag{9}$$

Such waves, when passing a parallel plate with the thickness d, compose a linearly polarized wave with an azimuth different from the original at an angle ρ when coming into vacuum. Matching the solutions at $z = d$, it is easy to get the value of this angle in radians as follows

$$\rho = \frac{k_0^2 \gamma}{2} d = \frac{\pi}{\lambda} |n_+ - n_-| \, d.$$

Note that ɣ has the dimensions of length, as it follows from (2). The Formula (9) gives us a regular rotatory power in rad/cm for $d = 1$ and λ expressed in cm.

So far, this is all what can be obtained from the system (5), as in the general case of oblique incidence of the wave. It is not possible to solve this system in some simple way [7].

ii) Let us make the following transformations: from the second equation of system (4) we obtain

$$H_x = \frac{1}{i k_0} E_y'. \tag{10}$$

Substituting this into the third equation of the same system, we obtain the following

$$H_y = \frac{1}{i k_0^3 \gamma} \left(E_y'' + k_y^2 E_y \right). \tag{11}$$

Then the magnetic components shall be substituted in the fourth equation, so

$$E_x = \frac{1}{k_0^4 \gamma \varepsilon_{xx}} \left[E_y'' + \left(k_y^2 + k_0^4 \gamma^2 \right) E_y \right]'. \tag{12}$$

Finally, value E_x shall be substituted in the first equation, where, taking into account (11), we obtain the following fourth order equation

$$\left(E_y'' \right)'' - \mathcal{A} E_y'' + \mathcal{B} E_y = 0 \tag{13}$$

where

$$\mathcal{A}=\frac{\varepsilon_{xx}}{\varepsilon_{zz}}k_z^2+k_y^2+k_0^4\gamma^2, \quad \mathcal{B}=\frac{\varepsilon_{xx}}{\varepsilon_{zz}}\left(k_y^2k_z^2-k_0^4k_x^2\gamma^2\right).$$

In the particular case of a non-gyrotropic anisotropic medium only diagonal elements in the matrix of the system (4) are nonzero. Then system (5) is transformed into the following two independent equations:

$$E_y''+k_y^2E_y=0, \quad E_x''+\frac{\varepsilon_{xx}}{\varepsilon_{zz}}k_z^2E_x=0 \tag{14}$$

for s-wave and p-wave, respectively. The elementary case of isotropic non-gyrotropic media, as noted by Landau [4], is degenerated because the equations for the s-wave and p-wave in (14) are identical.

The general solution of a fourth-order differential equation is a linear combination of the four particular solutions of the form

$$E_y=\sum\nolimits_{j=1}^{4}C_j\exp(\Lambda_jz),$$

where C_j are constants to be defined for a specific type of a problem, and Λ_j are the roots of the characteristic equation

$$\Lambda^4-\mathcal{A}\Lambda^2+\mathcal{B}=0.$$

Fortunately, the last equation is a biquadratic equation, and we get the roots in an elegant form

$$\Lambda_{1,2}^{\pm}=\pm i\sqrt{-\mathcal{A}/2\mp\sqrt{\mathcal{A}^2/4-\mathcal{B}}}=\pm iK_z^{\pm}.$$

In the case of an isotropic gyrotropic medium we get the following:

$$K_z^{\pm 2}=\frac{k_0^4\gamma^2}{2}+k_z^2\mp k_0^3\gamma\sqrt{\frac{k_0^2\gamma^2}{4}+\varepsilon}.$$

Hence, we obtain the dispersion equation since

$$K_z^{\pm 2}+k_x^2=k_0^2n_{\pm}^2$$

where $n_{\pm}$ is a refractive indices of two waves propagating in the same direction. Then, neglecting terms with γ^2, we obtain

$$n_{\mp}^2=\varepsilon\mp k_0\gamma\sqrt{\varepsilon}. \tag{15}$$

Let us also use the dispersion Equation (15) to show the importance of the gyrotropy indicator γ, which is in fact more important than the one obtained for the lr-polarizations. Using the equality

$$n_+^2-n_-^2=(n_++n_-)(n_+-n_-),$$

and the approximate equation $n_++n_-\approx 2\sqrt{\varepsilon}$ we obtain Formula (9).

It is seen from the above considerations that the field components E_y and H_x are related to each other in the same regular way, as for a non-gyrotropic medium according to (10). We may assume that the wave corresponding to them is an independent s-wave, while the p-wave depends on it according to (11) and (12), as it is for a gyrotropic medium. Based on that, we may consider our evaluations as performed in the quasi-basis of sp-polarization.

Let us show now a direct process of calculation and consider the reflection and transmission of a linearly polarized wave on a plane-parallel plate (film) with the boundaries $z=0$ and $z=d$. In a vacuum (medium-1), Equation (14) has the following solutions:

$$E_y=\exp\left(-ik_z^{(0)}z\right)+r_s\exp\left(ik_z^{(0)}z\right),$$
$$E_x=\exp\left(-ik_z^{(0)}z\right)+r_p\exp\left(ik_z^{(0)}z\right),$$

where $k_z^{(0)}=\sqrt{k_0^2-k_x^2}$, r_s and r_p are reflectivities of the s- and p-waves, respectively. The azimuth is 45°, so for the incident wave its magnitude is 1.

After passing through the plate, light gets in vacuum or in an isotropic medium (medium-2) with a dielectric constant ε_s, where solutions of Equation (14) can be written as

$$E_y=t_s\exp\left(-ik_z^{(s)}z\right), \quad E_x=t_p\exp\left(-ik_z^{(s)}z\right); \quad k_z^{(s)}=\sqrt{k_0^2\varepsilon_s-k_x^2}$$

where t_s and t_p are transmissivities of s- and p-waves, respectively. We obtain the rest of the field components H_x and H_y for medium-1 and medium-2 from (4) setting $\gamma = 0$.

Finally, for a most anisotropic and gyrotropic plate a main wave shall be selected as a solution of Equation (13):

$$E_y = \tau_1 \exp\left(-iK_z^- z\right) + \tau_2 \exp\left(-iK_z^+ z\right) + \rho_1 \exp\left(iK_z^- z\right) + \rho_2 \exp\left(iK_z^+ z\right),$$

where the constants τ_1, τ_2; ρ_1, ρ_2 correspond to the internal transmittance and reflectance, respectively. Then it is possible to express the fields H_x, H_y and E_x through E_y according to Formulas (10)–(12).

Now it is possible to show how to staple the fields at the boundary of the plate. Setting E_y, H_x, H_y and E_x equal to each other on the plate boundary with the medium-1 at $z = 0$ and on the border with the medium-2 at $z = d$, we obtain a linear system of algebraic equations in eight unknowns

$$\mathbf{SX} = \mathbf{C}, \tag{16}$$

where $\mathbf{S} = [s_{lm}]$

$$\mathbf{S} = \begin{bmatrix} 1 & 0 & -1 & -1 & -1 & -1 & 0 & 0 \\ k_z^{(0)} & 0 & K_z^- & K_z^+ & -K_z^- & -K_z^+ & 0 & 0 \\ 0 & -\dfrac{k_0}{k_z^{(0)}} & \dfrac{K_z^{-2}}{m_{23}m_{34}} & \dfrac{K_z^{+2}}{m_{23}m_{34}} & \dfrac{-K_z^{-2}}{m_{23}m_{34}} & \dfrac{-K_z^{+2}}{m_{23}m_{34}} & 0 & 0 \\ 0 & 1 & \dfrac{-iK_z^{-3}+iK_z^-\mu}{m_{23}m_{34}m_{41}} & \dfrac{-iK_z^{-3}+iK_z^-\mu}{m_{23}m_{34}m_{41}} & \dfrac{-iK_z^{-3}+iK_z^-\mu}{m_{23}m_{34}m_{41}} & \dfrac{-iK_z^{-3}+iK_z^-\mu}{m_{23}m_{34}m_{41}} & 0 & 0 \\ 0 & 0 & e_-^- & e_-^+ & e_+^- & e_+^+ & -\exp\left(-ik_z^{(s)}d\right) & 0 \\ 0 & 0 & -s_{23}e_-^- & -s_{24}e_-^+ & -s_{25}e_+^- & -s_{26}e_+^+ & K_z^{(s)}\exp\left(-ik_z^{(s)}d\right) & 0 \\ 0 & 0 & -s_{33}e_-^- & -s_{34}e_-^+ & -s_{35}e_+^- & -s_{36}e_+^+ & 0 & -\dfrac{k_0\varepsilon_s\exp\left(-ik_z^{(s)}d\right)}{K_z^{(s)}} \\ 0 & 0 & -s_{43}e_-^- & -s_{44}e_-^+ & -s_{45}e_+^- & -s_{46}e_+^+ & 0 & -\exp\left(-ik_z^{(s)}d\right) \end{bmatrix}$$

$\mathbf{X} = [r_s;\ \ r_p;\ \ \tau_1;\ \ \tau_2;\ \ \rho_1;\ \ \rho_2;\ \ t_s;\ \ t_p]$

is a column-vector of unknown coefficients,

$$\mathbf{C} = \left[-1;\ \ k_z^{(0)}/k_0;\ \ -k_0/k_z^{(0)};\ \ -1;\ \ 0;\ \ 0;\ \ 0;\ \ 0\right]$$

is the definite column-vector,

$$e_-^- = \exp(-iK_z^- d), \quad e_-^+ = \exp\left(-iK_z^+ d\right),$$
$$e_+^- = \exp\left(iK_z^- d\right), \quad e_+^+ = \exp\left(iK_z^+ d\right); \quad \mu = m_{23}m_{32} + m_{34}m_{43}.$$

For compact representation of the matrix $\mathbf{S}$ using recursion, terms $s_{23}, s_{24}, \dots s_{46}$ are matrix elements as defined above in lines 2–4.

Solving the system (16), we find the unknown coefficients, which form vector $\mathbf{X}$. Out of all the unknown coefficients we are more interested in the external reflection coefficients r_s and r_p, and transmissions t_s and t_p, through which we calculate the observable quantities, i.e., the rotation and depolarization:

$$\rho_r = \Psi = \arctan\left(|r_p/r_s|\right), \quad \delta_r = \Delta = \arg\left(r_p/r_s\right), \quad \rho_t = \arctan(|t_p/t_s|), \quad \delta_t = \arg\left(t_p/t_s\right),$$

where Ψ and Δ are ellipsometrics angles.

In the conclusion, we would like to present two examples, which illustrate the obtained new solution. The first example is the calculation for the well-studied quartz crystal, whose $|n_+ - n_-| = 6.6 \times 10^{-5}$ and rotatory power is equal to 188 deg/cm at the HeNe-laser wavelength $\lambda = 0.6328\,\mu\text{m}$ [8]. The ordinary and extraordinary refractive indices of quartz for this wavelength are $n_o = 1.54$, $n_e = 1.55$, respectively [9]. Consider a quartz plate thickness to show it as a gyrator and as a compensator. Known [10] that the thickness $\lambda/4$-plate is determined by the formula

$$d = \left|\frac{2m+1}{n_o - n_e}\right| \frac{\lambda}{4},$$

where m is an integer. We choose $m = 0$, $\lambda = 0.6328\,\mu\text{m}$, then $d = 15.82\,\mu\text{m}$. If the plate cut normal to the optical axis, it will operate as a gyrator. As can be seen from Figure 1 (line 1), at normal incidence depolarization $\delta_t = 0$, the wave at the exit from the plate is linearly polarized. The plane of polarization $\rho_t = 0.297\,\text{deg}$, which is exactly the rotatory power of quartz.

In addition, we note that the calculation shows that at normal incidence, the rotatory power is very weakly dependent on the refractive indices of the crystal. Of course, the refractive indices in the xy plane should be equal, i.e., crystal was cut out normal to the optical axis

In the second case, suppose that the optical axis is directed along the axis x, for example. At the exit of the plate light acquires a phase shift $-90\,\text{deg}$, i.e., it becomes circularly polarized. Rotation ρ_t naturally loses practical sense. Figure 1 shows a perfect agreement between the theoretical considerations and the experimental results.

The second example is from the ellipsometry of the thin films [11]. We considered a film obtained by vacuum deposition of chalcogenide glass As_2S_3 (the substrate is crystal KCl, $n_s = 1.488$ at $\lambda = 0.6328\,\mu\text{m}$). Previously, we already considered the anisotropy method described above for such films, but excluding gyrotropy [12]. This experiment confirms that gyrotropy is very weakly manifested in reflected light. As can be seen from Figure 2, only for a sufficiently large $\gamma \sim 10^{-3}\,\mu\text{m}$ corresponding to about gigantic gyrotropy, noticeable differences in the calculations are observed.

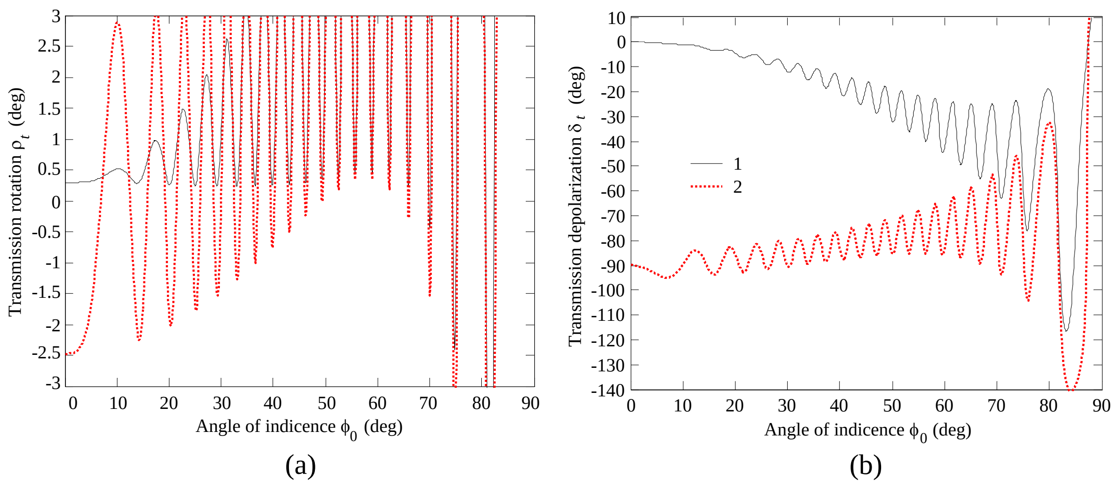

Figure 1. (a) The rotation angle ρ_t and (b) the depolarization angle δ_t for the quartz plate, thickness $d = 15.82\,\mu\text{m}$. Lines 1: $n_x = 1.54$, $n_y = 1.54$, $n_z = 1.55$. Lines 2: $n_x = 1.55$, $n_y = 1.54$, $n_z = 1.54$. Everywhere $\gamma = 6.6 \times 10^{-5}/k_0 \approx 6.6 \times 10^{-6}$ (μm).

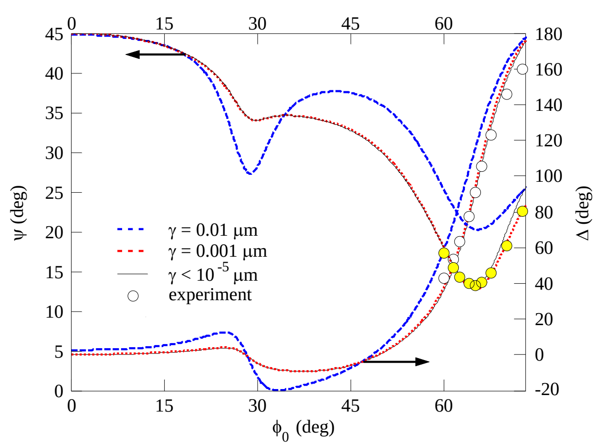

Figure 2. Ellipsometric angles Ψ and Δ as a function of the incidence angle ϕ_0 of thin film, refractive index $n_f = 2.453$, $d = 2.103\,\mu\text{m}$ at different γ.

ACKNOWLEDGMENT

I want to thank my colleague V. Yu. Loya for kindly providing me samples of thin films.

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