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Effective Impedance Method for *In situ* Ellipsometry Analysis of Magnetic Films

L.V. Panina[1,*], A.T. Morchenko[1], L.V. Kozhitov[1], P.A. Ryapolov[2]

[1] *National University of Science and Technology, MISIS, 4, Leninsky Ave., 119049 Moscow, Russia*
[2] *Department of Nanotechnology and Engineering Physics, Southwest State University, 305040 Kursk, Russia*

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The method of effective surface impedance is proposed and applied for *in situ* characterisation of magnetic structures. For any ellipsometry investigations a proper choice of a physical model is important for solving the inverse problem. Reasonable approximations used for *in situ* ellipsometry monitoring are assumptions of a constant rate of layer growth and stable optical parameters. Standard ellipsometry analysis requires the model response to be calculated from every layer in the structure. Errors from underlying layers propagate through the entire structure and accumulate. In this case a method of a pseudosubstrate is used which approximates the underlying structure as a single interface (so called virtual interface), rather than tracking the entire sample history. The virtual interface is placed at some level and growth is modelled on this interface with no knowledge retained for the underlying structure. There are various methods for describing the virtual interface. In this paper, the concept of the effective impedance is used which requires only three measurement data points and is convenient for combined investigation of optical and magneto-optical properties. The algorithm is based on the calculation of the characteristic matrix of the layer (Abeles matrix) and surface impedance of the virtual interface using two ellipsometric experimental data points. The method is successfully used to analyse Co / SiCo films.

Keywords: *In situ* ellipsometry**,** Magnetic films, Multilayers, Pseudosubstrate, Effective impedance.

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1. INTRODUCTION

Multilayered nanofilms consisting of transition metals, semiconductors and dielectrics have attracted a lot of interest because of their advanced applications in electronics as memory cells, logic gates in magnetic random access memories or read heads in hard disk drives. This research faces tremendous technological challenges to produce films with the required properties. Moreover, identically prepared films may show different properties. For example, tunnel junctions of the same composition often show different junction specific switching behaviour [1]. To understand the magnetic multilayer properties, the simultaneous study of structural, electronic and magnetic properties is required. Usually this is done by a combination of several different experimental techniques such as optical spectroscopy, spectroscopic ellipsometry, nuclear magnetic resonance, or neutron scattering. Generalised magneto-optical ellipsometry which combines Kerr spectroscopy and spectroscopic ellipsometry [2] allows an optical analysis of electronic and magnetic properties under exactly the same measurement conditions.

In situ characterization during the film growth or after film deposition would be preferable, especially in the case of the ultra thin films because the exposure of nanofilms to ambient can result in oxidation of the films and thus modification in their properties [3]. Successful application of *in situ* magneto-optical methods for characterisation of thin Co films obtained by electron beam evaporation was demonstrated in [4]. *In situ* characterisation also makes it possible to collect data during the multilayer film growth process. This provides access to various layers at different points during the deposition. This is equivalent to the benefits from multiple sample analysis, but applied to the same technological and environmental conditions.

Ellipsometry measures the change in polarization that occurs when a light beam is reflected from a sample. The polarization change itself is not generally the property of interest, but can be used to determine material properties such as thin film thickness, optical constants, and microstructure. Basic ellipsometry measurements produce two quantities (typically expressed as Ψ and Δ) at each wavelength and angle of incidence. Although certain wavelengths and angles are more sensitive to material properties, multiple measurements can contain equivalent information [5, 6]. While ellipsometry measurements are sensitive to both optical constants and film thickness, they are not a direct measurement. In a few simplified cases, the equations can be inverted to calculate optical constants or film thickness from measured Ψ, Δ data. Spectroscopic ellipsometry characterization is generally subject to the ‘inverse problem’ where the measurement can be predicted from a sample description, but sample properties cannot be directly calculated from the measured data. Regression analysis is commonly used to determine the best-fit results considering all acquired data simultaneously.

When *in situ* ellipsometry measurements are taken during thin film growth, the unknown sample properties are determined at each measurement point, when adequate information is available. Typically, thin layers require special techniques to determine both optical constants and thickness [5]. Standard ellipsometry analysis requires building the model based on the response from every layer in the structure. Errors from underlying layers may accumulate resulting in large deviations from a real structure. A pseudosubstrate with a single interface (virtual interface, VI) can approximate the underlying

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[*] lpanina@plymouth.ac.uk

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structure, instead of using a full multilayer model as shown in Fig. 1, where the VI intersects the fifth layer and the structure is modelled on this interface without tracking the response from the underlying layers.

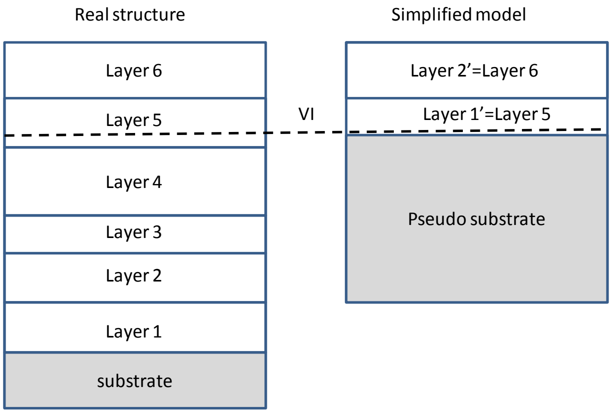

Fig. 1 – Comparison of real structure and simplified optical model obtained with the use of virtual interface. Pseudosubstrate is used to simplify *in situ* ellipsometry data analysis by approximating the underlying layers as a single interface

There are various methods for calculating a VI properties [7-9]. Here we will use a modified common pseudosubstrate approximation and use multiple time-points to allow a direct solution. It is proposed to characterise VI by two surface impedance parameters which are calculated using at least two ellipsometric data points and use them as intermediate variables to deduce the ellipsometric data obtained at VI (See Fig 2). The proposed approach can be used for thin magnetic films to simultaneously obtain optical and magneto-optical properties. The algorithm was successfully applied to characterise Co/Si/Co/glass structure.

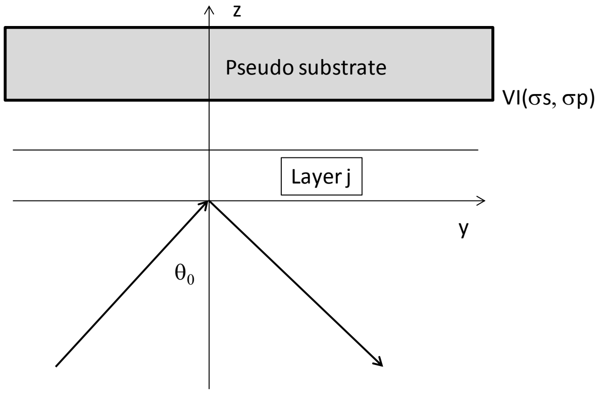

Fig. 2 – Schematics of the optical model for the virtual interface (VI) algorithm

Virtual interface is characterised by two components of the surface impedance σ_p and σ_s corresponding to *p*- and *s*-polarised waves:

$$\sigma_p = \frac{E_y}{H_x}, \qquad \sigma_s = \frac{E_x}{H_y} \tag{2}$$

The reflection parameters r_p and r_s, measured from pseudosubstrate for *p*- and *s*-waves are related to σ_p and σ_s as

$$r_s = \frac{\sigma_s q_{s0} - 1}{\sigma_s q_{s0} + 1}, \qquad r_p = \frac{\sigma_p + q_{p0}}{\sigma_p - q_{p0}} \tag{3}$$

Here

$$q_{s0} = n_0 \cos\theta_0, \qquad q_{p0} = \cos\theta_0 / n_0$$

θ_0 is the angle of incidence and n_0 is the refractive index of the medium of incidence. The ellipsometric parameter ρ is defined as

$$\rho = \tan\psi \exp(i\Delta) = \frac{r_p}{r_s} \tag{4}$$

The measurement of ρ gives the information about the properties of the VI which is characterised by two complex parameters σ_p and σ_s. These parameters can be calculated from two ellipsometric data points ρ_1 and ρ_2 which are measured for growing structure above the pseudosubstrate. The value ρ_0 obtained for the VI will be used to set the figure of merit for the determination of properties of the upper layers.

For this purpose, we relate the components of the electromagnetic field taken at some planes in the structure above VI to the components at VI plane in a usual form with the help of the characteristic matrices $\hat{M}_s$, $\hat{M}_p$:

$$\begin{pmatrix} E_x \\ H_y \end{pmatrix} = \hat{M}_s \begin{pmatrix} E_x(\mathrm{VI}) \\ H_y(\mathrm{VI}) \end{pmatrix}, \qquad \begin{pmatrix} H_x \\ E_y \end{pmatrix} = \hat{M}_s \begin{pmatrix} H_x(\mathrm{VI}) \\ E_y(\mathrm{VI}) \end{pmatrix} \tag{5}$$

In the case of *s*-polarisation, the magnetisation of the layers does not influence the wave propagation and the characteristic matrix is of the form:

$$\hat{M}_s = \prod \hat{M}_{sj}$$

$$\hat{M}_{sj} = \begin{pmatrix} \cos\left(\beta_j h_j\right) & -\dfrac{i}{q_{pj}} \sin\left(\beta_j h_j\right) \\ -i q_{pj} \sin\left(\beta_j h_j\right) & \cos\left(\beta_j h_j\right) \end{pmatrix} \tag{6}$$

$$q_{sj} = n_j \cos\theta_j, \beta_j = k_0 n_j \cos\theta_j, k_0 = \frac{2\pi}{\lambda} \tag{7}$$

Here n_j, θ_j, h_j are the refractive index, angle of refraction and thickness of layer *j* above VI, λ is the wavelength.

In the case of *p*-waves, and nonmagnetic layers equation (6) for $\hat{M}_{pj}$ holds with q_{sj} replaced by

$$q_{pj} = -\frac{\cos\theta_j}{n_j} \tag{8}$$

For magnetic layers in the linear approximation with respect to *Q*, the diagonal components of $\hat{M}_{pj}$ becomes:

$$M_{pj}^{11} = \cos\beta z - iQ m_x \tan\theta_j \sin(\beta z)$$
$$M_{pj}^{22} = \cos\beta z + iQ m_x \tan\theta_j \sin(\beta z)$$

Equations (5) can be written in terms of the surface impedances σ_s, σ_p and the reflection coefficients r_s, r_p from the topmost layer

$$A_s\begin{pmatrix}1+r_s\\(1-r_s)q_{s0}\end{pmatrix}=\widehat{M}_s\begin{pmatrix}\sigma_s\\1\end{pmatrix} \qquad (9)$$

$$A_p\begin{pmatrix}1+r_p\\-(1-r_p)q_{p0}\end{pmatrix}=\widehat{M}_p\begin{pmatrix}1\\\sigma_p\end{pmatrix} \qquad (10)$$

where A_s, A_p are the normalization parameters. Excluding these parameters from matrix equations (9), (10) yields

$$r_s=\frac{q_{s0}(M_s^{11}\sigma_s+M_s^{12})-(M_s^{21}\sigma_s+M_s^{22})}{q_{s0}(M_s^{11}\sigma_s+M_s^{12})+(M_s^{21}\sigma_s+M_s^{22})} \qquad (11)$$

$$r_p=\frac{q_{p0}(M_p^{11}+M_p^{12}\sigma_p)+(M_p^{21}+M_p^{22}\sigma_p)}{q_{p0}(M_p^{11}+M_p^{12}\sigma_p)-(M_p^{21}+M_p^{22}\sigma_p)} \qquad (12)$$

The ratio (12) to (11) gives the ellipsometric points. Taking two points from upper layers ρ_1, ρ_2, the virtual interface impedances can be calculated. In fact, this will produce two sets of solutions and without the third measurement (at virtual interface) it is not possible to decide which solution should be taken. It implies that the obtained solutions for the impedances can be used to calculate from equations (3) the ellipsometric parameter ρ_0 at the interface. For this calculation, the experimental points ρ_1, ρ_2, together with the refractive index and thickness of the topmost films are needed. Thus, the introduced impedances are intermediate variables which are needed to define the figure of merit γ at each wavelength λ_n

$$\gamma=\sum_{\lambda_n}(\rho_{0theor}(\rho_1,\rho_2,n_1,n_2,h_1,h_2,\lambda_n)-\rho_{0\exp})^2 \quad (13)$$

The values of n_1, n_2, h_1, h_2 are used as fitting parameters to minimise γ. Therefore, we constructed the figure of merit using the information about the film structure only above the pseudosubstrate.

2. VI ALGORITHM FOR MAGNETIC FILMS

The phenomenological description of optical and magneto-optical parameters is based on the matrix form of the permittivity. Considering that the plane of incidence is the y, z plane and the magnetisation is along the x-axis (equatorial Kerr effect), the permittivity of isotropic magnetic layer has the form

$$\hat{\varepsilon}=\varepsilon\begin{pmatrix}1&0&0\\0&1&-iQm_x\\0&iQm_x&1\end{pmatrix} \qquad (14)$$

Here Q is the magneto-optical constant and m_x is the x-directional cosine of the magnetisation. In this case, the p (H_x, E_y, E_z) and s (E_x, H_y, H_z) polarised waves remain the eigenfunctions and the consideration is convenient to make in terms of the Abeles matrices (see for details [10]). The configuration of the structure is shown in Fig. 2.

3. TESTING THE ALGORITHM WITH Co / Si / Co STRUCTURE

The proposed algorithm was tested using the experimental data obtained at deposition of Co / Si / Co film on a glass substrate. The films were prepared in UHV chamber by magnetron sputtering method on oxidized, (001)-oriented Si substrate. The ellipsometric data were measured after the deposition of the first 10 nm thick Co film which was used as the virtual interface data ρ_0, then after the deposition of Si film as ρ_1 and after the deposition of the top Co film as ρ_2, as shown in Fig. 3a. The data ρ_0 were also used to define the refractive index of Co layer to perform calculations in (13). The best fitting ($\rho_{0theory}$) was obtained with the thicknesses of Si layer of 4 nm and the thickness of Co layer of 9.5 nm. The definition of the layer thickness from the deposition rate is 5 nm and 10 nm, respectfully. Therefore, the VI algorithm was comfortably used to characterised the magnetic multilayers.

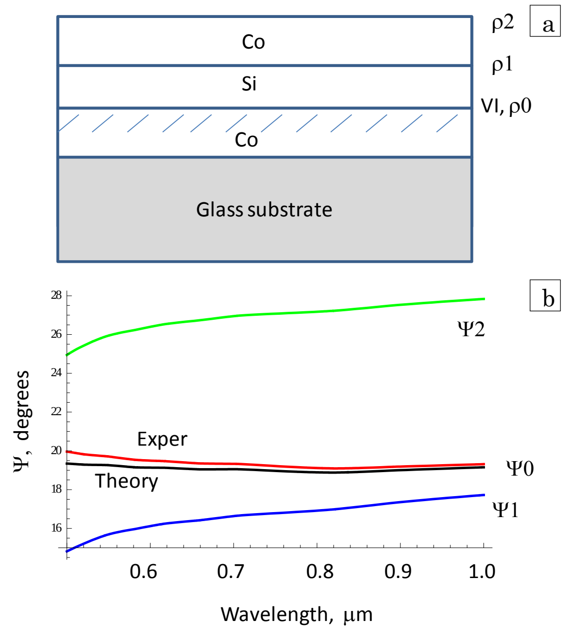

Fig. 3 – Tested multilayer film structure (a) and ellipsometric angles Ψ and Δ as a function of the wavelength (b). The angle of incidence is 70 degrees. The refractive index of Si was taken as 3.44904 + 2271.88813exp(– λ / 0.058304) + 3.39538exp (– λ / 0.30384) [11]

4. CONCLUSIONS

The approach of a pseudosubstrate and virtual impedance (VI) for *in situ* characterisation of magnetic multilayers is developed in terms of effective surface impedance. The virtual interface is placed at some level and growth is modelled on this interface. Direct calculation of the impedances requires two ellipsometric points and the third point at VI is used to set the figure of merit. The method is successfully used to analyse Co / Si / Co films.

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