Modeling of Light Scattering by Penetrable Particle Inside a Film Based on Discrete Sources Method

H.Yu. Eremina and A.G. Sveshnikov

Physics Faculty, Moscow Lomonosov State University,
Vorobyev' Hills, 119899, Moscow, Russia

Abstract

Our paper is dedicated to analysis of the light scattering by the particle in a film deposited on silicon substrate. The numerical method of investigating the complete mathematical problem is based on the Discrete Sources Method (DSM). It allows us to consider the electromagnetic wave scattering by different kinds of obstacles. The dependence of light scattered intensity by particles of different kind of material, size and location, and for different incidence angles are presented. The validity of total integral response is discussed.

1. INTRODUCTION

Advanced semiconductor devices are characterized by increased circuit density. Successful manufacturing of such devices requires decreasing the size of defects appearing under the different stages of technology process. In particular, it is necessary to detect a particle inside a thin film deposited on silicon wafer surface when lithography process is used. For this purpose the surface scanners, using a laser source of light, are the most efficient. The detection of particle is based on detailed investigation of light scattered by the particle. Experimental analysis of such kind of defects is expensive and rather complex because of weak signal of the scattered light. To expand the current detection ability one must have efficient mathematical model and computer simulation technique. Such mathematical model is based on complete system of Maxwell equations with strict boundary conditions and radiation conditions at infinity.

In our paper DSM is applied to investigation of P/S light scattering by a particle in a film deposited at the substrate. In the framework of DSM an approximate solution to the scattering problem is represented as a finite linear combination of the fields of elementary sources – dipoles and multipoles with unknown amplitudes. The approximate solution satisfies Maxwell equations everywhere inside and outside the scatterer, boundary conditions at the surface of the film and radiation conditions analytically. As it is well known to approximate the exact solution outside of the scatterer it is sufficient to approximate the boundary conditions at the scatterer's surface in the mean-square norm. Thus, the scattering problem is reduced to the approximation of the boundary

conditions of the exciting field at the scatter's surface. So, we are able to construct relations to determine Discrete Sources (DS) amplitudes.

In the case of stratified structure it is possible to construct dipoles and multipoles field satisfying the field transmission conditions at the films' boundaries. It allows to fit all conditions of the scattering problem analytically except the boundary condition at the particle surface. In this case the dipoles and multipoles fields are constructed on the base of Weyl-Sommerfeld integrals.

In case of axial symmetrical obstacle one is able to reduce the surface approximation problem to the sequence of one-dimensional approximation problems at the particle profile. To accomplish this we set DS at the symmetry axis. Then the approximate solution becomes a finite sum of a Fourier harmonics with respect to an azimuth variable φ. By expanding the external excitation in terms of a Fourier series with respect to φ-angle we transform the two-dimensional approximation problem into sequence of one-dimensional approximation problems at the surface element of the particle for each azimuth harmonic.

There are various approaches one can use to determine the DSM amplitudes. A more reliable technique that generates stable results is the point-matching the Fourier harmonics at a finite set of points of the surface element. As was outlined in [4], more stable results can be produced if one uses an over-determined system of linear equations.

2. MATHEMATICAL FORMALISM

Let the incident linear polarized plane wave $\{\mathbf{E}^0, \mathbf{H}^0\}$ has an incident angle γ with respect to the normal of a plane boundary Ξ_f of upper half space D_0, and film D_f. Plane Ξ_1 is the boundary of the film and a substrate. Let the axially symmetric particle D_1, having a smooth boundary ∂D be situated entirely into the film between planes Ξ_f and Ξ_1 of the thickness d, that its symmetry axis coincides with the normal to Ξ_1. Let us introduce a Cartesian coordinate system $Oxyz$ with its origin point located on the substrate and direction of the Oz axis coincides with the symmetry axis of the particle. The mathematical model can be formulated as the following boundary-value problem (BVP):

$$\nabla \times \mathbf{H}_t = ik\varepsilon_t \mathbf{E}_t; \qquad \nabla \times \mathbf{E}_t = -ik\mu_t \mathbf{H}_t \quad \text{in } D_t, \quad t = 0, f, 1, i, \tag{1}$$

$$\begin{aligned}\mathbf{n}_p \times \left(\mathbf{E}_i(p) - \mathbf{E}_f(p)\right) = 0,\\ \mathbf{n}_p \times \left(\mathbf{H}_i(p) - \mathbf{H}_f(p)\right) = 0,\end{aligned} \quad p \in \partial D, \tag{2}$$

$$\begin{aligned}\mathbf{e}_z \times \left(\mathbf{E}_0(p) - \mathbf{E}_f(p)\right) = 0,\\ \mathbf{e}_z \times \left(\mathbf{H}_0(p) - \mathbf{H}_f(p)\right) = 0,\end{aligned} \quad p \in \Xi_f, \tag{3}$$

$$\begin{aligned}\mathbf{e}_z \times \left(\mathbf{E}_f(p) - \mathbf{E}_1(p)\right) = 0,\\ \mathbf{e}_z \times \left(\mathbf{H}_f(p) - \mathbf{H}_1(p)\right) = 0,\end{aligned} \quad p \in \Xi_1, \tag{4}$$

attenuantion/radiation conditions at infinity ($z \neq 0,d$) (5)

Here $\mathbf{n}_p$ is a unit normal to ∂D, and $\{\mathbf{E}_t, \mathbf{H}_t\}$ is a total field in appropriate area. The particle surface is assumed to be smooth enough, $\partial D \subset C^{(1,\alpha)}$, and the media parameters satisfy the conditions $\operatorname{Im} \varepsilon_t, \mu_t \leq 0$ (the time dependence $\exp\{i\omega t\}$). Then BVP (1-5) has a unique correct solution.

Before we construct an approximate solution of the scattered waves we need to solve the plane wave $\{\mathbf{E}^0, \mathbf{H}^0\}$ difraction problem by the layered structure. As it is well-known, this solution may be represented in an explicit form. Let's designate an obtained field $\{\mathbf{E}_t^0, \mathbf{H}_t^0\}$, $t = 0, f, 1$.

The solution should account for the axial symmetry and polarization of the incident wave. To satisfy (3) we use the Green's tensor components to construct the DS fields. Thus, Hertz vectors for vector multipoles have the following expression:

$$\mathbf{A}_{mx}^{e,h} = \mathbf{e}_x g_m^{e,h} - \mathbf{e}_z f_{m+1} \cos\phi, \quad \mathbf{A}_{my}^{e,h} = \mathbf{e}_y g_m^{e,h} - \mathbf{e}_z f_{m+1} \sin\phi,$$

where index e corresponds to the electrical type of vector multipoles having components $\mathbf{e}_x, \mathbf{e}_y$ and h corresponds to magnetic types. The appropriate azimuthal term

$$g_m^{e,h}(q, w_n) = \int_0^\infty J_m(\lambda\rho) v_{11}^{e,h}(z, w_n, \lambda) \lambda^{1+m} d\lambda, \tag{6}$$

$$f_m(q, w_n) = \int_0^\infty J_m(\lambda\rho) v_{31}^{e,h}(z, w_n, \lambda) \lambda^{1+m} d\lambda, \tag{7}$$

where J_m is cylindrical Bessel function, the point $q=(\rho,z)$ is located in the half-plane ϕ=const, and the multipoles are located at the symmetry axis $w_n \in Oz$ inside D_i. In this case for spectral functions $v_{11}^{e,h}(z,w_n,\lambda), v_{31}^{e,h}(z,w_n,\lambda)$ the following representations hold:

$$v_{11}^{e,h}=\begin{cases} A_{11}^{e,h}(\lambda,w_n,d)\exp\{-\eta_0(z-d)\} & z>d, \\ \dfrac{\exp\{-\eta_f|z-z_0|\}}{\eta_f}+B_{11}^{e,h}\exp\{-\eta_f(d-z)\}+ & \\ \qquad +C_{11}^{e,h}\exp\{-\eta_f z\} & d>z>0, \\ D_{11}^{e,h}\exp\{\eta_1 z\} & z<0, \end{cases}$$

$$v_{31}^{e,h}=\begin{cases} A_{31}^{e,h}(\lambda,w_n,d)\exp\{-\eta_0(z-d)\} & z>d, \\ B_{31}^{e,h}\exp\{-\eta_f(d-z)\}+C_{31}^{e,h}\exp\{-\eta_f z\} & \\ & d>z>0, \\ D_{31}^{e,h}\exp\{\eta_f z\} & z<0. \end{cases} \tag{8}$$

Here $\eta_t^2=\lambda^2-k_t^2$, $k_t^2=k^2\varepsilon_t\mu_t$. Except those, spectral functions satisfy the following conditions at the boundaries *z= 0, d*:

$$\begin{aligned} &\left[v_{11}^e\right]=\left[1/\mu\left(\frac{dv_{11}^e}{dz}\right)\right]=0, && \left[1/\mu\left(v_{33}^e\right)\right]=\left[1/\varepsilon\mu\left(\frac{v_{33}^e}{dz}\right)\right]=0, \\ &\left[v_{11}^h\right]=\left[1/\varepsilon\left(\frac{dv_{11}^h}{dz}\right)\right]=0, && \left[1/\varepsilon\left(v_{33}^h\right)\right]=\left[1/\varepsilon\mu\left(\frac{v_{33}^h}{dz}\right)\right]=0, \\ &\left[1/\varepsilon\mu\left(\frac{v_{31}^e}{dz}\right)\right]=-[1/\varepsilon\mu]v_{11}^e, && \left[1/\mu\left(v_{31}^e\right)\right]=0, \\ &\left[1/\varepsilon\mu\left(\frac{v_{31}^h}{dz}\right)\right]=-[1/\varepsilon\mu]v_{11}^h, && \left[1/\varepsilon\left(v_{31}^h\right)\right]=0, \end{aligned} \tag{9}$$

From relations (9) it is easy to show, that inside a film the relation $v_{31}^e=v_{31}^h$, $d\geq z\geq 0$ takes place.

We'll build an approximate solution, using DSM [1]. The representation of total field inside the particle is based on regular functions, whose singularities are located at infinity [2]

$$\mathbf{A}^i_{mx} = g^i_m(q, w_n)\mathbf{e}_x, \qquad \mathbf{A}^i_{my} = g^i_m(q, w_n)\mathbf{e}_y,$$

$$g^i_m(q, w) = j_m(k_i R_{qw}) \times (k_i \rho / R_{qw})^m$$

where j_m – spherical Bessel function and $w_n \in Oz$. It's easy to see that $\rho / R_{qw} = \sin\theta_{qw}$, where θ_{qw} is an angle of spherical coordinate system with its origin point *w*. Thus, g^i_m functions may be represented as

$$g^i_m(q, w) = j_m(k_i R_{qw}) P^m_m(\cos\theta_{qw}) \frac{k_i^m}{(2m-1)!!}.$$

where P^m_m are joined functions of Legendre. Now it is easy to notice, that functions

$$G^i_m(q, w) = g^i_m(q, w) \begin{Bmatrix} \sin m\varphi \\ \cos m\varphi \end{Bmatrix}$$

satisfy the homogeneous Helmholtz equation $\Delta G^i_m + k_i{}^2 G^i_m = 0$ everywere in the finite area R^3.

We'll build approximate solution outside and inside D_i, which takes into account not only rotational symmetry of the scatterer, but also simultaneously polarization of external excitation [3].

Let us consider *P* polarized plane wave (the S-case was discussed in [6]), having angle θ_0 with *Oz* axis. Using the DSM methodology [3], we'll have the following combinations of potentials taking into account the external field polarization

$$\begin{cases} \mathbf{A}^e_{\upsilon f} := \mathbf{A}^e_{mx} \cos m\phi - \mathbf{A}^e_{my} \sin m\phi, \\ \mathbf{A}^h_{\upsilon f} := \mathbf{A}^h_{mx} \sin m\phi + \mathbf{A}^h_{my} \cos m\phi, \end{cases} \begin{cases} \mathbf{A}^e_{\upsilon i} := \mathbf{A}^i_{mx} \cos m\phi - \mathbf{A}^i_{my} \sin m\phi, \\ \mathbf{A}^h_{\upsilon i} := \mathbf{A}^i_{mx} \sin m\phi + \mathbf{A}^i_{my} \cos m\phi, \end{cases} \quad (10)$$

$\upsilon = \{m, n\}$ – multi-index with range of change: $0 \le m \le M$, $1 \le n \le N$, here M is a maximum number of the Fourier harmonics, and N – multipoles number, the same for all values of m. Let's denote v_0, Y $(Y = \{M, N\})$ the lower and upper values of multi-index. Besides we introduce vector potentials for vertical dipoles. The component with subscript 33 (i.e. σ) answers for vertical dipoles in Green tensor

$$\mathbf{A}_{n0}^{e} = \sigma^{e}(q, w_n)\mathbf{e}_z, \quad \mathbf{A}_{ni}^{e} = g_0^{i}(q, w_n)\mathbf{e}_z, \quad \sigma^{e} = g_0^{h}(q, w_n) \tag{11}$$

We suppose that external and internal electromagnetic fields create a dual vector $\mathbf{F}^{\eta} = \left\{\mathbf{E}^{\eta}, \mathbf{H}^{\eta}\right\}^{T}$, $\eta = e, h$, and refer the following differential forms

$$D_1 = \begin{pmatrix} i/k\varepsilon_\tau\mu_\tau & \nabla\times\nabla\times \\ -1/\mu_\tau & \nabla\times \end{pmatrix}, \qquad D_2 = \begin{pmatrix} i/\varepsilon_\tau & \nabla\times\nabla\times \\ i/k\varepsilon_\tau\mu_\tau & \nabla\times \end{pmatrix}$$

For convenience we shall use contracted notation for fields, constructing the approximate solution

$$\mathbf{F}_{\upsilon t}^{e} = D_1\mathbf{A}_{\upsilon t}^{e}, \qquad \mathbf{F}_{\upsilon t}^{h} = D_2\mathbf{A}_{\upsilon t}^{h} \tag{12}$$

than the representation for the approximate solution of BVP (1-5) for P polarized field is

$$\mathbf{F}_t^{Y} = \sum_{\upsilon=\upsilon_0}^{Y}\left\{p_\upsilon^t\mathbf{F}_{\upsilon t}^{e} + q_\upsilon^t\mathbf{F}_{\upsilon t}^{h}\right\} + \sum_{n=1}^{N} r_n^t\mathbf{F}_{nt}^{e}, \tag{13}$$

Where the last sum corresponds to vertical dipole sources.

So, the approximate solution of BVP (1-5) for the scattered field $\{\mathbf{E}_t^s, \mathbf{H}_t^s\}$, in $D_t, t = 0, f, 1$ and total field in D_i (13), which in addition takes into account polarization of an exciting plane wave satisfy:

- Maxwell equations in $D_{0,f,1,i}$;
- radiation and attenuation conditions in $D_{0,f,1}$;
- transmission conditions at the boundaries $\Xi_{f,1}$.

So, the representation (13) satisfies all conditions of BVP (1-5), except conditions at the particle surface.

By virtue of a completeness of a system of multipoles [2] and theirs orthogonality for two types of polarizations [3] the approximate solution (13) of the scattering problem (1-5) can be obtained with any degree of accuracy.

3. NUMERICAL SCHEME

We shall follow the scheme [1], underlining only the main differences. As it was already marked, the approximate solution (13) satisfies all conditions of BVP (1-5), except conditions at particle surface. So, the determination of unknown DS amplitudes is conducted just from conditions on ∂D surface.

It is convenient to divide the algorithm of amplitudes determination into several stages. As the sources are localized on the symmetry axis or in an appropriate part of a complex plane [3], the approximate solution (13) of BVP (1-5) is a final linear combination of Fourier harmonics on azimuth variable ϕ. Therefore at the first stage we decompose tangent components of electrical and magnetic fields of exciting plane waves in a Fourier series with respect to ϕ using representation for a plane wave of the following kind

$$\exp\{\pm i\varpi\cos\phi\} = \sum_{m=0}^{\infty}(2-\delta_{0m})(\pm i)^m J_m(\varpi)\cos m\phi\,, \qquad (14)$$

here $\varpi = k_f\,\rho\sin\theta_0$. As the representation for fields $\{\mathbf{E}_t^{\mathrm{Y}},\mathbf{H}_t^{\mathrm{Y}}\}$ (13) has a form of a finite linear combination of Fourier of harmonics, the DS amplitudes determination is reduced to determination of amplitudes vector for harmonics (i.e. at the fixed value of azimuth harmonics m number). Therefore the surface approximation is reduced to one-dimensional approximation on element $\Im$ of surface ∂D.

For solution of this problem we use the method of collocations, sewing together the azimuth harmonics at a collocation points set $\{\chi_\ell\}_{\ell=1}^{L} \subset \Im$, and solving the obtained in such a way over-determined system of linear equations.

The numerical algorithm of calculation of Weyl-Sommerfeld integrals (6-7) is applied to determine the limiting field values outside the particle surface at collocation points.

It is possible to construct computing algorithm so, that for determination of DS amplitudes both for P, and for S polarization it is sufficient to use the pseudo-inversion of the same matrix [1].

For scattered field intensity calculation at infinity it is necessary to have the scattered pattern. It is determined by following form:

$$\mathbf{E}(\mathbf{r})\Big/\left|\mathbf{E}^0(\mathbf{r})\right| = \frac{\exp\{-ik_0 r\}}{r}\mathbf{F}(\theta,\phi) + O(1\big/r^2), \quad r \to \infty.$$

In our case for scattered pattern it is possible to use asymptotic representations of Weyl-Sommerfeld integrals as it is made in [4].

Then the final formulas for the patterns don't contain the Weyl-Sommerfeld integrals, and can be easily calculated after the determination of unknown DS amplitudes. Then for θ,ϕ - a component of scattering diagram in case of P polarization we have

$$F_\theta^P = \frac{ik_0}{\varepsilon_0}\sum_{m=0}^{M}\cos(m+1)\phi(ik_0\sin\theta)^m\sum_{n=1}^{N}\{p_{nm}^0[G_{nm}^e\cos\theta + ik_0\sin^2\theta F_m]$$
$$+ q_{nm}^0 G_{nm}^h\} - \frac{ik_0}{\varepsilon_0}\sin\theta\sum_{n=1}^{N} r_n^0 G_{n0}^h\frac{\mu_0}{\mu_f},$$

$$F_\phi^P = -\frac{ik_0}{\varepsilon_0}\sum_{m=0}^{M}\sin(m+1)\phi(ik_0\sin\theta)^m\sum_{n=1}^{N}\{p_{nm}^0 G_{nm}^e + q_{nm}^0[G_{nm}^h\cos\theta + \tag{15}$$
$$+ ik_0\sin^2\theta F_m]\},$$

here spectral functions $G_{nm}^{e,h}, F_m$ are the following

$$G_{nm}^{e,h} = ik_0\cos\theta\exp\{ik_0 d\cos\theta\}A_{11}^{e,h}(k_0\sin\theta, w_n, d)$$
$$F_{nm} = ik_0\cos\theta\exp\{ik_0 d\cos\theta\}A_{31}(k_0\sin\theta, w_n, d)$$

Thus, the elements of the Green's Tensor in a far zone and the components of the scattering diagrams both for P and for S polarization do not contain the Weyl-Sommerfeld integrals. Therefore after determination of the unknown DS amplitudes for computing of the scattering characteristics it is sufficient to calculate combination of elementary functions only (15).

4. COMPUTER SIMULATING RESULTS

In the present section the main attention will be concentrated on the analysis of computer simulating results correspond to the wavelength of an exciting plane wave equal to 0.488mkm. On Figures the distribution of intensities (in mkm^2 units) of the scattered light in the incident plane (plane, originated by half-planes $\phi=0°$ and $\phi=180°$) depending on a scattering angle and dependence of total integral response from the scattered angle

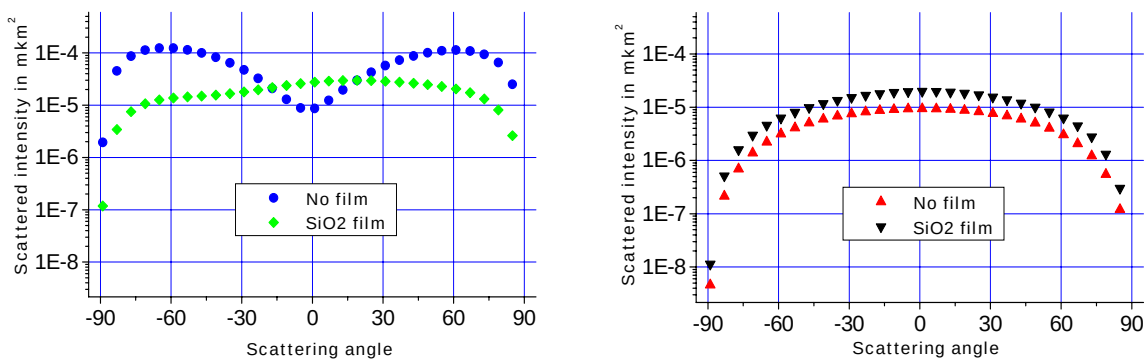
$$I^{P,S}(\theta,\phi)=\left|F_{\theta}^{P,S}(\theta,\phi)\right|^2+\left|F_{\phi}^{P,S}(\theta,\phi)\right|^2$$

are demonstrated.

We will concern particles of different kind of material, different size and location, and the different incidence angles. We also concerned the ratio of energy flux throught the particle surface to the energy, radiated into the upper halfspace for different particles. Fig.7 illustrates these results.

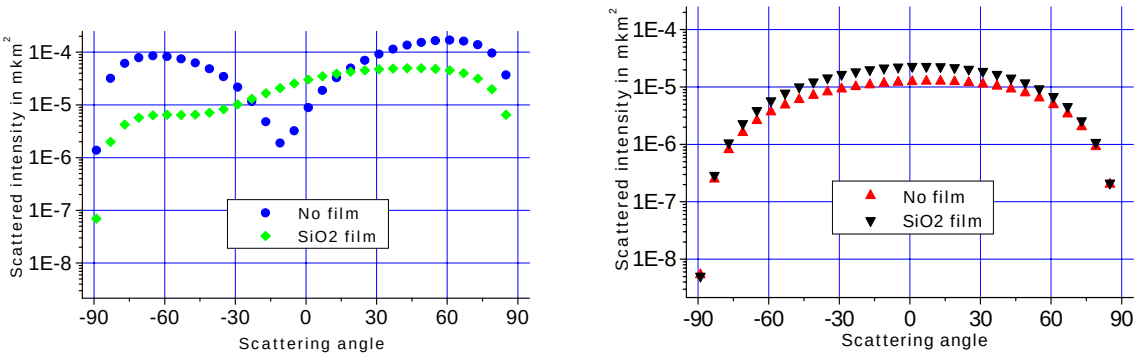
On Figs.1,2,4(a),5,6 the dependence of scattered light intensities on the scattering angle for incident angle 65° of the plane wave are shown.

Figs.3,4(b) illustrates the dependence of total integral response on incident angle for different particles.



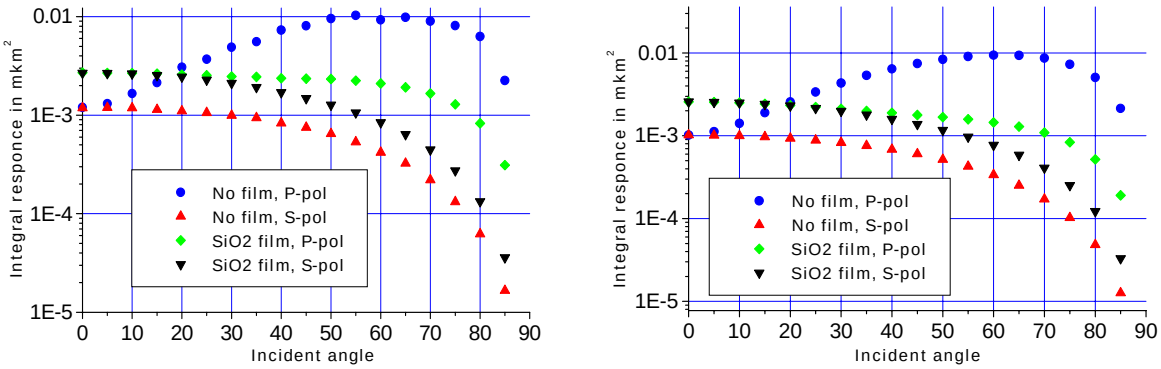
(a) **(b)**

Figure 1. Fe particle D=0.10mkm, at Si substrate in case of no film and SiO_2 film thickness=0.20mkm, **(a)** P-polarized, **(b)** S-polarized.



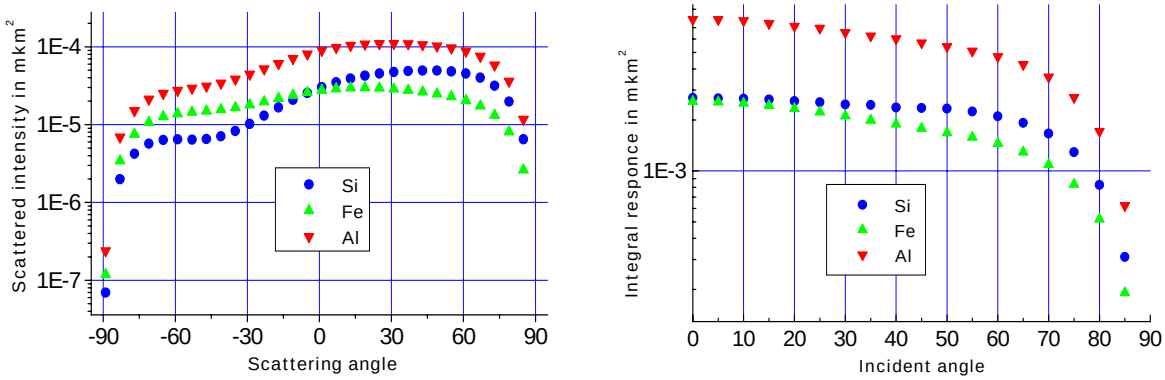
(a) **(b)**

Figure 2. Si particle D=0.10mkm, at Si substrate in case of no film and SiO_2 film thickness=0.20mkm, **(a)** P-polarized, **(b)** S-polarized.



(a) **(b)**

Figure 3. Si (a) and Fe (b) particles D=0.10mkm, at Si substrate in case of no film and SiO_2 film thickness=0.



(a) **(b)**

Figure 4. Particles D=0.10mkm, in SiO_2 film thickness =0.20mkm, at Si substrate.

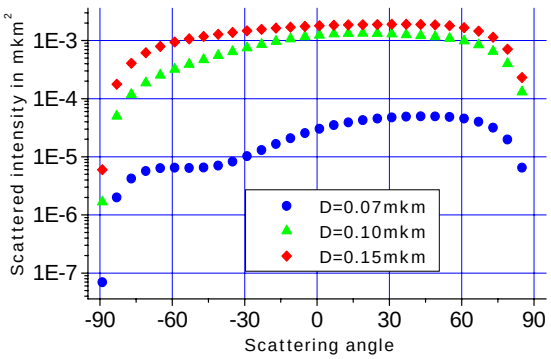


Figure 5. Si particles in SiO_2 film thickness=0.20mkm, at Si substrate.

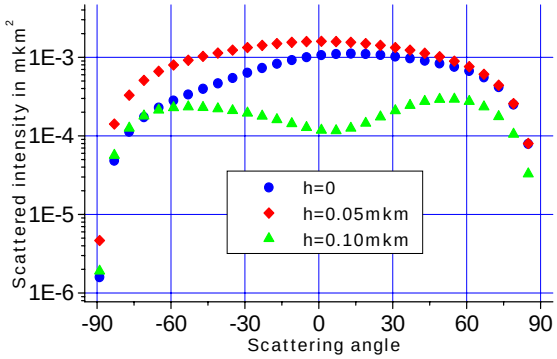
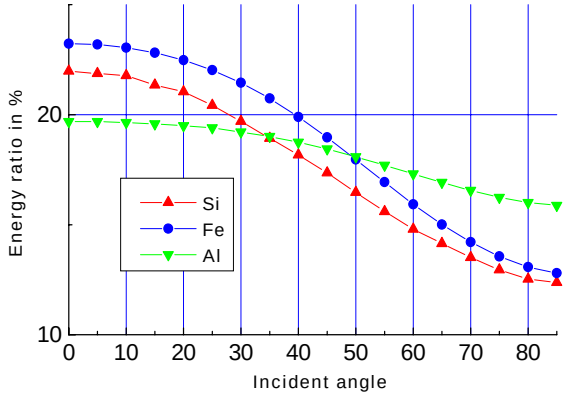
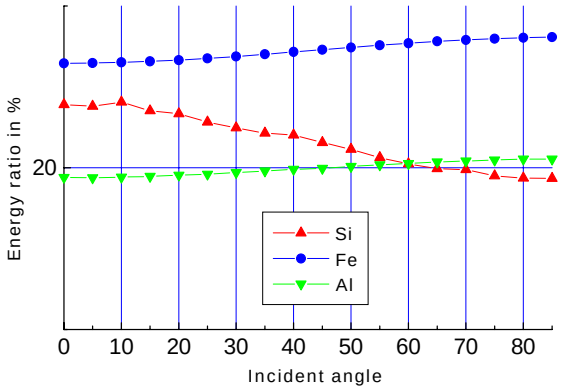


Figure 6. Al particle D=0.10mkm, in SiO_2 film, at different heights from Si substrate.



(a)



(b)

Figure 7. Particles D=0.10mkm, in SiO_2 film thickness=0.20mkm, at Si substrate.

5. CONCLUSION

1. The Total Integral Response (TIR) of P-polarized light smoothly decreases in presence of SiO2 film. In case of no film the TIR of P-polarized light have a maximum at incident

angle approximately 65 degrees. As to the S–polarized light, it's TIR smoothly decreases in all cases.

2. In the absence of the film the difference of P and S polarizations is much strongly.
3. Scattered intensity of P-polarized light in cases of SiO2 film presence and in the case of no film have a principal different view.
4. P-polarized light intensity strongly depends on the particle height and dimentions.

The a posteriori estimate of obtained results error was conducted by computation of discrepancy of boundary conditions at surface in l_2 norm. In presented below results the relative error does not exceed 2-3%.

REFERENCES

[1] Eremin Yu.A., Orlov N.V.: Simulation of Light Scattering from Particle upon Wafer Surface. Appl. Opt. **35** (1996).33, 6599-6605.

[2] Eremin Yu.A., Sveshnikov A.G.: *Method of Discrete Sources in Electromagnetic Scattering Problems*. M. MSU, (1992).

[3] Eremin Yu.A., Orlov N.V., Sveshnikov A.G. The Analysis of Complex Diffraction Problems by the Discrete-Source Method. Comput. Maths Math. Phys., **35** (1995) 6, 731-743.

[4] Eremin Yu.A., Sveshnikov A.G.: The Discrete Sources Method for Investigating Three-Dimensional Elecrtomagnetic Scattering Problems. Electromagnetics. **13** (1993) 1, 1-22.

[5] Orlov N.V., Eremin Yu.A.: Identification of Silicon Wafer Defects: Axi-Symmetrical Model. Proceedings of the 1-rd Workshop on Electromagnetic and Light Scattering: Theory and Applications, May 27-28, 1997, Moscow, Russia, pp.129-134.

[6] Eremina H.Yu., Sveshnikov A.G.: Analysis of Light Scattering by Particle Inside a Layer via Discrete Sources Method. Moscow University Physics Bulletin. Allerton Press, Inc. N1. 1999 (accepted for publication).