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OPTICS AND SPECTROSCOPY

ANALYSIS OF SCATTERING PROPERTIES OF OXIDE PARTICLES ON A MULTILAYER SUBSTRATE

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Polarized light scattering by oxide microparticles located on a film-coated substrate is analyzed. To carry out computer simulation, the method of discrete sources is extended. The effect of the film and oxide layer on the particle scattering properties is studied.

INTRODUCTION

Rapid progress in refining micro- and nanoelectronic circuits requires that special cleanliness should be ensured at all stages of the bulk-effect integrated circuits production process. The manufacture of defect-free circuits becomes a top-priority task of modern technologies. Since most defects are beyond the capabilities of visual inspection, flaw detection in such circuits makes use of surface scanners containing a laser source of polarized light and a system of collectors for the radiation scattered by the defect. It is known that in the manufacture of bulk-effect integrated circuits, blanks are silicon substrates. To produce the integrated circuit structure, the substrate is subjected to a lithographic process. An important stage in this process is the deposition of a film on the polished silicone substrate and detection of contaminating microparticles on the film surface by the surface scanner [1].

This work is devoted to modeling the processes of polarized laser radiation scattering by an oxide particle located on the surface of a multilayer structure (film–substrate). The basis for the development of a mathematical model of the scattering process is the method of discrete sources [2] that was successfully used previously to study the scattering properties of particles on and pits in substrates [3, 4].

MATHEMATICAL MODEL OF AN OXIDE PARTICLE ON A FILM-COATED SUBSTRATE

We describe the mathematical statement of the problem in hand. Let $\{\mathbf{E}^0, \mathbf{H}^0\}$ be the field of a linearly polarized plane electromagnetic wave incident at an angle of θ_0 to the normal on the flat interface Ξ_f between the air D_0 and the film D_f. An axially symmetric homogeneous particle D_i coated with a layer D_l and having smooth coaxial boundaries $\partial D_{i,l}$ is located on the surface Ξ_f of the film d in thickness. The film is bounded by the parallel planes Ξ_f and Ξ_1, the plane Ξ_1 separating the film from the substrate D_1. We will assume that the symmetry axis of the oxide particle coincides with the direction of the external normal to Ξ_1. Let us introduce a Cartesian coordinate system with its origin on the plane Ξ_1 and the Oz-axis directed along the symmetry axis of the particle. In that case, the mathematical statement of the problem has the form

$$\nabla\times\mathbf{H}_\xi = ik\varepsilon_\xi\mathbf{E}_\xi;\ \ \nabla\times\mathbf{E}_\xi = -ik\mu_\xi\mathbf{H}_\xi \quad \text{in}\ \ D_\xi,\ \ \xi=0,f,1,i,l,$$

$$\begin{aligned}
&\mathbf{e}_z\times\begin{cases}(\mathbf{E}_0(p)-\mathbf{E}_f(p))=0,\\ (\mathbf{H}_0(p)-\mathbf{H}_f(p))=0,\end{cases} \quad p\in\Xi_f,\\
&\mathbf{e}_z\times\begin{cases}(\mathbf{E}_f(p)-\mathbf{E}_1(p))=0,\\ (\mathbf{H}_f(p)-\mathbf{H}_1(p))=0,\end{cases} \quad p\in\Xi_1,\\
&\mathbf{n}_i\times\begin{cases}(\mathbf{E}_i(p)-\mathbf{E}_l(p))=0,\\ (\mathbf{H}_i(p)-\mathbf{H}_l(p))=0,\end{cases} \quad p\in\partial D_i,\\
&\mathbf{n}_l\times\begin{cases}(\mathbf{E}_l(p)-\mathbf{E}_0(p))=0,\\ (\mathbf{H}_l(p)-\mathbf{H}_0(p))=0,\end{cases} \quad p\in\partial D_l,
\end{aligned} \tag{1}$$

plus the emission (or decay) conditions for the scattered fields at infinity.

Here $\{\mathbf{E}_\xi,\mathbf{H}_\xi\}$ is the total field in the corresponding region; $\mathbf{e}_z$ is the unit vector of the normal to the interface $\Xi_{1,f}$ of the multilayer medium; and $\mathbf{n}_{i,l}$ are the normals to the surfaces $\partial D_{i,l}$. We note that in the region D_0 the total field includes both the incident and the reflected plane wave, as well as the filed scattered by the particle. We also notice that, as far as its statement is concerned, the problem under consideration is close to that studied in detail in [5]. However, the presence of the additional oxide layer D_l coating the particle D_i, as well as a different position of the scattering particle with respect to the layer make the implementation of the general approach suggested in [2] substantially different.

Before constructing an approximate solution for scattered fields, we solve the problem of diffraction of the field $\{\mathbf{E}^0,\mathbf{H}^0\}$ of plane polarized wave by the multilayer air–film–substrate structure. It is known [6] that such a solution can be written in explicit form. Let it be $\{\mathbf{E}^0_\xi,\mathbf{H}^0_\xi\}$, $\xi=0,f,1$. We now construct the approximate solution of boundary-value problem (1) for the scattered field $\{\mathbf{E}^s_\xi,\mathbf{H}^s_\xi\}$ in D_ξ, $\xi=0,f,1$, and for the total field in $D_{i,l}$ on the basis of the method of discrete sources [2]. The essence of this method is that the fields are represented in the form of finite linear combinations of the fields of multipoles satisfying the set of Maxwell equations in the regions D_ξ, $\xi=0,f,1,i,l$, the conditions at infinity for the scattered field in $D_{0,f,1}$, and also the conjugation conditions for the tangential field components everywhere on $\Xi_{f,1}$. In that case, the solution of scattering boundary-value problem (1) is reduced to the determination of the unknown discrete source amplitudes solely from the conjugation conditions at the interfaces $\partial D_{i,l}$ between the different media of the multilayer particle, which assume the form

$$\begin{aligned}
&\mathbf{n}_i\times(\mathbf{E}_i-\mathbf{E}_l)=0, \\
&\mathbf{n}_i\times(\mathbf{H}_i-\mathbf{H}_l)=0 \qquad \text{at}\ \ \partial D_i,\\
&\mathbf{n}_l\times(\mathbf{E}_l-\mathbf{E}^s_0)=\mathbf{n}_l\times\mathbf{E}^0_0,\\
&\mathbf{n}_l\times(\mathbf{H}_l-\mathbf{H}^s_0)=\mathbf{n}_l\times\mathbf{H}^0_0 \qquad \text{at}\ \ \partial D_l.
\end{aligned} \tag{2}$$

We recall that ∂D_i is the internal boundary and ∂D_l is the layer–air interface. Here $\{\mathbf{E}^0_0,\mathbf{H}^0_0\}$ is the total field of the incident and reflected plane waves in D_0. Consequently, diffraction problem (1) is reduced to the solution of problem (2) of approximation of the field $\{\mathbf{E}^0_0,\mathbf{H}^0_0\}$. Such a problem can be solved by following the general theory of the method of discrete sources. Let us describe in a sketchy manner only the main points.

1. Our representation of the external field in D_0 is based on multipole sources satisfying the conjugation conditions for the fields on the planes $\Xi_{f,1}$. In that case, the structure of the fields is defined by the Green tensor of the multilayer medium, whose elements have the form presented in [5, 7]. Application of the Green tensor of the multilayer medium in constructing the scattered fields is the central point of the method, which allows all possible interactions between the particle and the plane-layer medium to be taken into account.

2. Since the interfaces $\partial D_{i,l}$ are axially symmetric and have a common axis normal to the substrate surface, it is reasonable to go over from joining problem (2) for the fields on $\partial D_{i,l}$ to the consecutive solution

of the problems of conjugation on the generatrices $\mathfrak{I}_{i,l}$ of the surfaces of revolution $\partial D_{i,l}$ for the Fourier harmonics of the fields in the azimuthal variable [3]. By specially selecting sources in the form of multipoles located on the symmetry axis, one can represent the fields in the form of a finite sum of the Fourier series in the azimuthal variable [3].

3. We represent the total field inside the particle (in D_i) on the basis of regular functions whose singularities are at infinity [2], the total field inside the layer D_l being constructed in the form of a sum of "outgoing" and "incoming" waves [2].

4. What is more, an approximate solution is constructed so as to take into consideration not only the scatterer axial symmetry, but the incident plane wave polarization [5] as well.

COMPUTATIONAL ALGORITHM

Consider the scheme of the computational algorithm. As noted above, the approximate solution constructed on the basis of the method of discrete sources satisfies all the conditions of boundary-value problem (1), except for conjugation conditions (2). For this reason, the unknown amplitudes of the discrete sources are determined so as to approximately satisfy conjugation conditions (2) in the appropriate functional norm [2]. The algorithm for finding the amplitudes can conveniently be subdivided into several stages. The approximate solution is a finite linear combination of Fourier harmonics in the azimuthal variable φ. At the first stage, therefore, we expand the tangential electric and magnetic field components of the exciting plane waves into a Fourier series in the azimuthal external excitation variable. As a result, the surface approximation is reduced to the approximation of the fields on the generatrices $\mathfrak{I}_{i,l}$ of the multilayer particle. At the next stage of finding the azimuthal amplitude components of the discrete sources use is made of the generalized collocation method, which makes it necessary to solve an overdetermined linear system for each azimuthal harmonic. The azimuthal amplitude components of the discrete sources are determined as a normal pseudosolution of overdetermined linear systems [7]. As distinct from [5], conditions (2) are conditions of conjugation on two different planes, namely, ∂D_i and ∂D_l, which substantially increases the order of overdetermined linear systems and gives rise to additional difficulties in the numerical implementation of the algorithm if the specified accuracy of the final result is to be retained.

The above-described scheme of the method of discrete sources makes it possible to organize computations so as to ensure that the scattering characteristics be calculated for all angles of incidence and two basic types of polarization (P and S). The model developed also enables one to make a posterior estimate of the error of the approximate solution obtained by calculating the residual of conjugation conditions (2) on the surface of the particle in the root-mean-square norm.

To calculate the scattered field intensity at infinity, it is necessary to have the scattering diagram in D_0. To find its concrete form, it is sufficient to use the asymptotic representations for the Weyl–Zommerfeld integrals, as done in [3]. In that case, we will have the same representations for the scattering diagram components as in [5]. Hence it follows that the Green tensor elements in the far-field region and, consequently, the scattering diagram components contain no integrals. Therefore, once the unknown amplitudes of the discrete sources are determined, the scattering characteristics can be determined by calculating the combination of elementary functions only. This circumstance makes it possible to analyze in detail such scattering characteristics as the scattering intensity and the integrated scattering cross section, i.e., the scattering intensity integrated within the limits of a solid angle Ω. It should be noted that most surface scanners use either mirror collectors or lenses to collect the scattered radiation within some solid angles, and so the integrated scattering cross section is a most adequate model for the collector system of a surface scanner.

NUMERICAL RESULTS

The range of parameters of the films used in practice is governed by their direct purpose. As a rule, the film thickness is varied between a few tens and a few hundreds of nanometers. The contaminating particles that can get on the film surface fall within a wide, though limited, variety of substances. Their diameter is much smaller than the laser radiation wavelength used (and, naturally, hundreds of times smaller than the laser spot diameter, which makes the above plane wave model an adequate external excitation model). At present, surface scanners can detect particles equal in volume to a ball up to 0.06 μm in diameter (what we have in mind are polystyrene latex particles [1]), the laser wavelength used most frequently being $\lambda = 0.488$ μm. Such small particles are frequently referred to as the Rayleigh particles and modeled by spherical balls of equal volume.

In this work, the main scattering characteristics being studied are the scattering intensity and the integrated scattering cross section calculated in the solid angle range $\Omega = \{0 \le \theta \le 80$ deg, $0 \le \varphi \le 360$ deg$\}$. We will conventionally call it the total scattering cross section (its dimension, μm^2, coincides with the dimension of the scattered radiation intensity). The posterior estimate of the accuracy of the approximate solution, based on the satisfaction of conjugation conditions (2), allows us to conclude that the relative error of the results presented below is no more than 5% in the uniform metric.

The prime objective of our investigation is to find out whether the main characteristics of contaminating particles that get onto the substrate are retained in the presence of the film and the oxide layer. It was found in [7] that the surface scanner resolution can be best improved at the excitation angle of -65 deg ($\theta_0 = 65$ deg, $\varphi = 180$ deg). Figure 1 shows the relationship between the scattering intensity and the scattering angle for a spherical particle with outside diameter $D = 0.07$ μm consisting of a copper core (refractive index $n = 1.143 - 2.536j$) and a CuO shell ($n = 2.53 - 0.7j$) 0.006 μm in thickness located on a silicon substrate ($n = 4.37 - 0.08j$). It can be seen that, as in the case of homogeneous particle, an inclined incidence and P-type polarization are preferable. As noted in [7], a characteristic indication of scattering by a particle is the presence of a dip in the vicinity of the normal to the substrate. As seen from Fig. 1, this holds true for oxide particles as well.

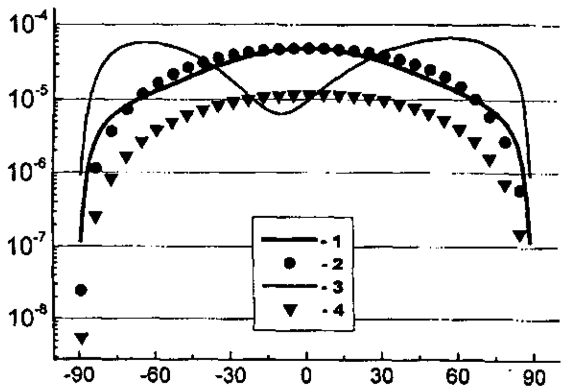

Fig. 1

Scattering intensity as a function of the scattering angle for a spherical copper particle 0.07 μm in outside diameter coated with a CuO layer with a thickness of $d = 0.003$ μm and located on a Si substrate: angle of incidence $\theta_0 = 0$, P-type (curve *1*) and S-type (curve *2*) polarization; angle of incidence $\theta_0 = -65$ deg, P-type (curve *3*) and S-type (curve *4*) polarization.

It was suggested [7] that particles should be identified by their total scattering cross section, for, as distinct from pits in the substrate, the total scattering cross section for P-type polarization increases within the range of scattering angles close to the normal. Figure 2 presents the calculation results for the total scattering cross sections of aluminum and copper oxide particles. As in the case of homogeneous particles, the total scattering cross section for P-type polarization grows as the angle of incidence is increased. The maximum in the region of $\theta_0 \cong 65$ deg makes it possible to determine the optimum angle providing for the maximum energy scattered into the upper half-space. It should be noted, at the same time, that the presence of the oxide layer may lead not only to the reduction of the scattered radiation intensity; Fig. 3 illustrates an "abnormal" rise of the intensity with the increasing thickness of the oxide layer.

Let us now demonstrate how the scattering characteristics change in the presence of the film. We consider SiN ($n = 2.0$) as the film material frequently used in practice. It is known that the presence of the film, which, as a rule, causes no perceptible damping, gives rise to various resonance effects. Figure 4

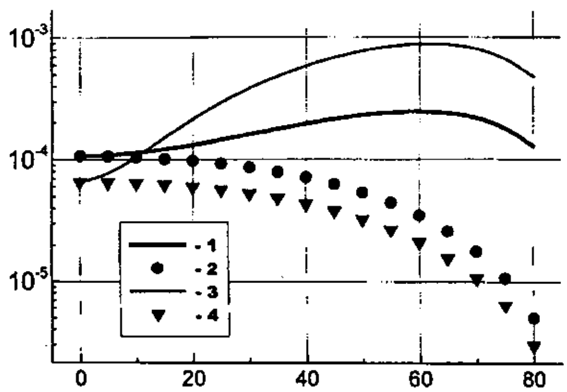

Fig. 2

Total scattering cross section as a function of the angle of incidence for an oxide particle 0.07 μm in diameter (oxide layer thickness $d = 0.003$ μm): copper particle, P-type (*1*) and S-type (*2*) polarization; aluminum particle, P-type (*3*) and S-type (*4*) polarization.

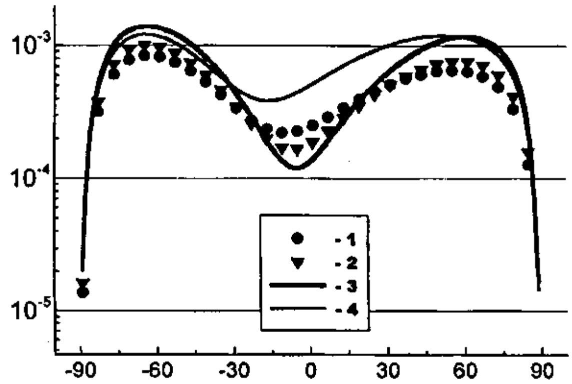

Fig. 3

Scattering intensity for an aluminum particle at $\theta_0 = -65$ deg and P-type polarization: pure aluminum particle with a diameter of (*1*) 0.1 μm and (*4*) 0.11 μm and aluminum oxide particle with a diameter of (*2*) 0.0025 μm and (*3*) 0.005 μm.

presents scattering intensities for an aluminum oxide particle located on films varying in thickness. As one can see from Fig. 4, at the film thickness $d = 0.20$ μm, the scattered field intensity substantially changes its structure. In this case, there is no characteristic dip that is observed in the case of particles on the substrate. This effect is characteristic of the multilayer medium film–substrate itself and is independent of the particle material. At the same time, in the case of resonance in the plane-parallel structure, the integrated scattering characteristics, specifically the total scattering cross section, keep behaving as before, which is illustrated in Fig. 5.

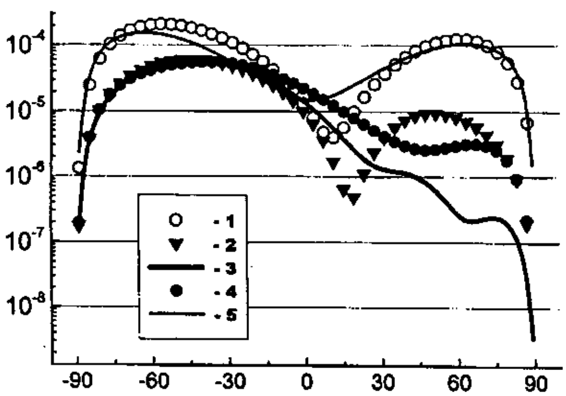

Fig. 4

Scattering intensity for an aluminum particle 0.07 μm in diameter coated with an oxide layer ($d = 0.003$ μm) and located on a SiN film ($\theta_0 = -65$ deg, P-type polarization): film thickness is equal to (*1*) 0.25 μm, (*2*) 0.21 μm, (*3*) 0.2 μm, (*4*) 0.19 μm, and (*5*) 0.15 μm.

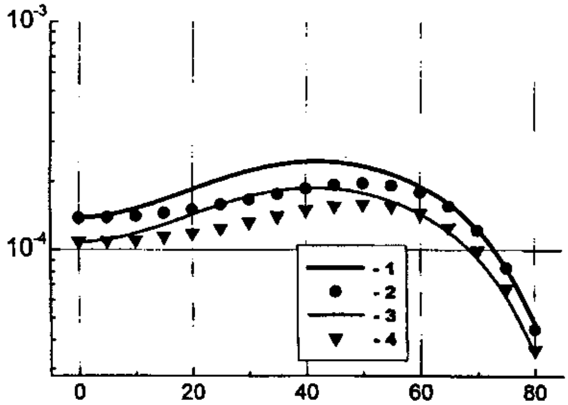

Fig. 5

Total scattering cross section for an aluminum particle 0.07 μm in diameter located on a SiN film 0.2 μm in thickness: pure aluminum particle, (*1*) P-type polarization and (*2*) S-type polarization; aluminum oxide particle, (*3*) P-type polarization and (*4*) S-type polarization.

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REFERENCES

1. J. Baliga, *Semicond. Intern.*, no. 4, p. 64, 1997.
2. Yu.A. Eremin and A.G. Sveshnikov, *Method of Discrete Sources in Electromagnetic Diffraction Problems* (in Russian), Moscow, 1992.
3. Yu.A. Eremin, N.V. Orlov, and A.G. Sveshnikov, *Matem. Modelirovanie*, no. 10, p. 113, 1996.
4. Yu.A. Eremin, N.V. Orlov, and A.G. Sveshnikov, *Matem. Modelirovanie*, no. 8, p. 110, 1997.
5. E.Yu. Eremina and A.G. Sveshnikov, *Vestn. Mosk. Univ. Fiz. Astron.*, no. 1, p. 12, 1999.
6. N.V. Grishina, *Opt. Spektr.*, vol. 80, no. 1, p. 123, 1996.
7. N.V. Grishina, Yu.A. Eremin, and A.G. Sveshnikov, *Fund. Prikl. Matem.*, vol. 4, no. 3, p. 889, 1998.

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