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Physics Procedia 23 (2012) 49 – 52

Physics Procedia

Asian School-Conference on Physics and Technology of Nanostructured Materials (ASCO-NANOMAT 2011)

Determination of structural parameters of the Fe-Si-system by spectral ellipsometry method

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Abstract

Limitation of the thin homogeneous layers with sharp interfaces model for the structure Si(100)/FeSi$_2$(grain) in solution the inverse problem of ellipsometry in the visible spectral range is shown. A new model of random distribution of thin disks for describing the real structure of the sample is designed. The results of the model optimization are confirmed by AFM.

Keywords: spectral ellipsometry; silicides; atomic force microscopic

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1. Introduction

During the formation of fine thin film on the substrate surface many processes occur at the surface (for example: adsorption of atoms on the surface, crystallization, sublimation of atoms from the surface, island growth [1]) need to be under the control. In this regard method of reflection ellipsometry acquired special relevance, it has a high surface sensitivity and in the spectral range of visible light has almost no damage of the sample. In this study the analysis of the most effective methods of solution the inverse problem of spectral ellipsometry was performed. The new model of the surface that provides the best fitting to the

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doi:10.1016/j.phpro.2012.01.013

ellipsometric data has been developed. For example a single crystal Si substrate and $FeSi_2$ islands have been considered.

2. Experiment

The measured ellipsometric spectra provides parameters *Ψ* and *Δ* included in the basic equation of ellipsometry

$$\rho \equiv tg\psi \cdot e^{i\Delta} = \frac{R_p}{R_s} \tag{1}$$

where R_p, R_s are the complex reflection coefficients for the two components of elliptically polarized light.

The inverse problem is solved with a linear regression analysis to optimize the structural parameters of the optical model of the sample surface. As the function of minimizing in the linear regression analysis, the standard deviation of the sample used:

$$\sigma = \frac{1}{M}\left\{\sum_{j=1}^{M}\left|\rho_{ex}(h\nu_j) - \rho_{cal}(h\nu_j)\right|^2\right\}^{\frac{1}{2}} \tag{2}$$

where M is a number of experimental points, and the values ρ_{ex} and ρ_{cal} are measured and calculated ratio of Fresnel coefficients.

Measurements of the parameters *Ψ* and *Δ* have been carried out ex situ with the high-speed spectral ellipsometer "Spectroscan" [2] in wavelength range 250 - 900 nm. We use a single crystalline silicon substrate with crystallographic orientation (100) and 2x1 reconstructed surface. Its surface has been covered at 150 ° C by the 2 nm iron layer with thermal evaporation in ultrahigh vacuum.

Construction of an optical model was carried out to increase its information content and a decrease the standard deviation. The simplest model is a thin uniform film of iron with sharp interface on the semi-infinite silicon substrate. As concerns geometric properties of the surface (roughness, shape of inhomogeneities), this model does not provide any information. When using a multilayer optical model with homogeneous sublayers and sharp interfaces between them, the optimization problem is complicated, but also an opportunity to reveal a nonuniform distribution of certain materials of the specimen height appears. Calculating the effective permittivity of a mixture of materials in a single sublayer the Likhteneker equation is used [3]:

$$\varepsilon_{eff} = \prod_{i=1}^{N} \varepsilon_i^{q_i} \tag{3}$$

where N is a number of components; ε_i is a permittivity of the i-th component, and q_i is a volume fraction of the i-th component.

Multilayer model allows to simulate arbitrary geometric shape of inhomogeneities on the surface, if such inhomogeneity function of the volume concentration of material height is set. However, this model cannot take into account the nonhomogeneous distribution of the individual grains.

The random distribution of flat grains on the surface were identified also in this sample by AFM [4] (Fig. 1(a)). The height of these grains is smaller than the wavelength of light, but the diameter, and especially the average distance between the grains more than the wavelength of light. Therefore, for this sample one cannot use the model of homogeneous films with sharp borders.

The model of uniform distribution of the inhomogeneous in height disks and their surrounding homogeneous dielectric film [5] for the calculation of nonoverlapping parts of the sample surface with different Fresnel coefficients was designed (Fig. 1(b)).

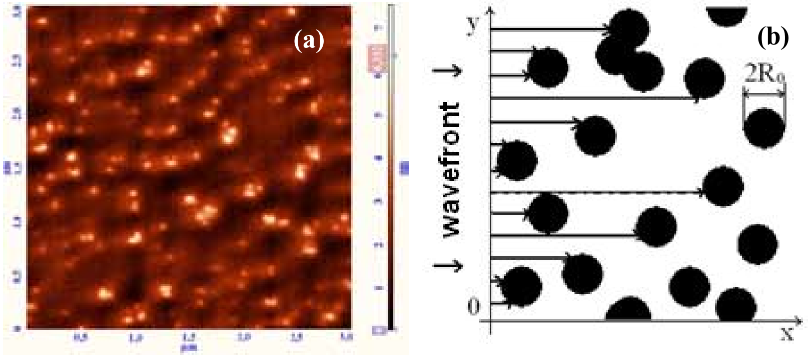

Fig.1. AFM scan of the sample surface 3x3 μm (a) and the model of random distribution of thin disks and the thin homogeneous film with the inclusion (b)

$$R_{p,s} = r_{01p,s} + \frac{\left(1 - r_{01p,s}{}^{2}\right)}{r_{01p,s} \cdot r_{12p,s} + \exp[2 i \delta]} \cdot \left(r_{12p,s} - r_{12p,s}{}^{m+2} \cdot \left(-r_{01p,s}\right)^{m+1} \cdot \exp[-2 i \delta (m+1)]\right) \qquad (4)$$

where $r_{ijp,s}$ are Fresnel coefficients of corresponding interfaces for p – and s – light polarization, δ is a phase thickness.

For equidistant thin disks:

$$m = \left\lfloor \frac{\pi R_0 \sqrt{1-\gamma}}{8 d \gamma} \right\rfloor \qquad (5)$$

For the homogeneous film with inclusions:

$$m = \left\lfloor \frac{\sqrt{1-\gamma}}{4 n R_0 d \gamma} \right\rfloor, \qquad \gamma = \frac{N_0}{N_1} \sin \varphi_0 \qquad (6)$$

where N_0, N_1 are refractive indices of the external environment and of the substance of the film or disks; R_0, n are radius and density of the surface distribution of disks; d is height of the corresponding element.

Optimization of the new model is done by the fitting height, diameter and shape of grains (in form of thin disks), their chemical composition, and also height and material of a homogeneous film.

3. Results and discussions

Optimizing the structural parameters of the model uniformly distributed thin disks the minimum value of standard deviation $9.6 \cdot 10^{-5}$ was found, that is almost 10 times less than for single-layer model of iron on silicon. The fitting performed in the wavelength range from 250 to 550 nm. According to the Fe–Si phase diagram [6] there is stable $FeSi_2$ phase at 150 °C. So we have used as the material of individual disks in our model – $FeSi_2$.

In spectral dependence of the measured and calculated values difference of *Δ* was seen in the wavelength increase. This is a feature of the ellipsometry method, when the parameter *Δ* and porosity of surface are increasing simultaneously. This effect partially decided by Effective Model [7].

The parameters of the optical model and the parameters of the AFM data in Table 1 are given in the table.

Table 1. Parameters of model

Method	Average disk height, (nm)	Average disk radius, (nm)	Density, (μm^{-2})	Coverage, (%)
Atomic Force Microscopic	3.5 ± 0.2	145 ± 6	14.1 ± 0.1	28.0 ± 0.1
Spectral Ellipsometry	5.1 ± 0.1	96 ± 1	9.4 ± 0.1	26.9 ± 0.2

The difference in AFM and Spectral Ellipsometry methods for height, density and radius of grains is a consequence of model unreality, for example, the presence of stoichiometric gradient in Si–$FeSi_x$ interface.

4. Conclusions

In this study, structural analysis of the sample surface of Fe-Si system has been performed by the spectral reflection ellipsometry. We obtain that at the surface there are individual disks (truncated cones of $FeSi_2$), surrounded by homogeneous film SiO_2.

Founded structural parameters from ellipsometry are consistent with AFM data. Designed optical model and method of optimization of structure can be used as a simple and fast alternative to various forms of microscopy.

Acknowledgements

This work was supported by project 4.1 of the OFN RAS, project 27.10 of the Presidium RAS, integration project 22 of SBRAS and DVO RAS, the FCP NK-179P/GK P1464, the Federal Program “Research and scientific-pedagogical personnel of Innovative Russia” for 2009–2013.

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