OPTICAL PROPERTIES OF NANOSTRUCTURED LAYERS ON SILICON

Stanislav Jurečka

Institute of Aurel Stodola, University of Žilina, Nálepku 1390,
03101 Liptovský Mikuláš, Slovakia
E-mail: jurecka@lm.uniza.sk

Received 30 April 2017; accepted 05 May 2017

1. Introduction

Nanostructured layers on silicon (Si) surface are formed for an achievement of the light reflectance suppression. Low spectral reflectance is important for improvement of the conversion efficiency of solar cells and for other optoelectronic applications. Effective method of forming of nanostructured layers with ultralow reflectance in a broad interval of wavelengths has been developed in Osaka University. It is based on metal assisted etching of Si. Si surface immersed in HF and H_2O_2 solution is etched in contact with the Pt mesh roller and the structure of the mesh is transferred on the etched surface (surface structure chemical transfer method, SSCT) [1-4]. The nonuniform dissolution of Si during the SSCT treatment forms porous nanocrystalline layers with gradient of layer density [5]. Ultralow spectral reflectance of the SSCT structure results from the depth gradient of material density increasing with the distance from the surface.

In this work we study optical properties of the SSCT layers. Density gradient in the layer structure is solved in our approach by representing of the nanostructured layer by a sublayer system. Dielectric function of each sublayer in this system is modelled by the Maxwell Garnett effective media approximation. Spectral reflectance of superposition system is computed by the Abeles scattering matrix formalism based on constructed dielectric functions [6].

2. Experimental part

The nanostrucured layers were formed on flat Si surface by the SSCT method. Microstructure of the SSCT layer is determined by the prolongation of etching time. The thicknesses of formed layers were determined by the transmission electron microscope JEOL EM-3000F with the incident electron energy of 300 keV. The spectral reflectance of formed structure was determined by using a JASCO V-670 UV–VIS spectrometer with an integrating sphere.

Tab. 1. *Nanostructured SSCT samples.*

Sample	**Etching time [s]**
SSCT 10	10
SSCT 20	20
SSCT 30	30

3. Results and discussion

In Fig. 1 the TEM image of the SSCT layer etched for 25 seconds is shown. From the TEM image the thickness value 250 nm of the SSCT layer was estimated. In Fig. 2 the spectral reflectance ***R*** of the SSCT layers is shown. Reflectance decreases drastically in a broad interval of wavenumbers in comparison to the flat Si surface.

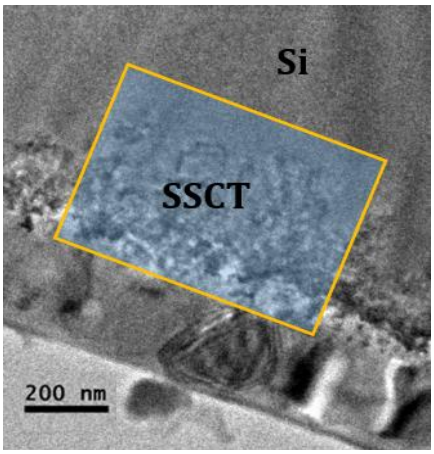

Fig. 1: *TEM image of the SSCT structure. SSCT layer is marked by a frame.*

The density of SSCT layer increases with the depth due to the etching mechanism. For the density graded materials the reflectance decreases exponentially with the thickness of reflecting structure [7]. For evaluation of the thickness *d* dependence of spectral reflectance we computed $R(d,\lambda)$ values by

$$R(d,\lambda)=R_{Si}(\lambda)e^{-cd/\lambda} \tag{1}$$

where $R_{Si}(\lambda)$ is spectral reflectance of flat Si surface.

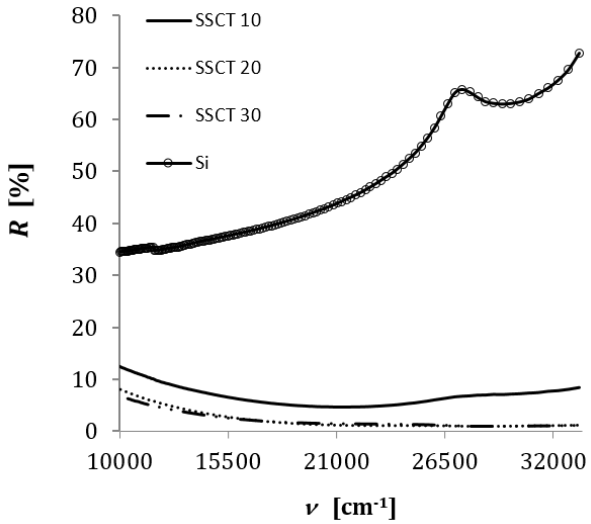

Fig. 2: *Spectral reflectance **R** of nanostructured SSCT layers formed on Si surface.*

In Fig. 3 plot of normalized reflectance $R(d,\lambda)/R_{Si}(\lambda)$ in semilog scale for the SSCT 20 structure is shown. Linear part of this function corresponds to exponential behaviour of normalized reflectance and show presence of the density gradient in the SSCT layer. Therefore we expect gradual changes of dielectric function with the thicknesses of the SSCT layers. In analysis of the optical properties of studied layer we usually create theoretical model of the dielectric function by using Drude-Lorentz (DL) theory [8]. DL model describes the optical response of a set of damped harmonic oscillators and response of unbound free charge carriers. Spectral reflectance $R(\lambda)$ is computed by using DL proposed dielectric function. To obtain acceptable $R(\lambda)$ theoretical model of the SSCT layer a large number of DL oscillators have to used. After adding more and more oscillators to the model function the estimation of the initial values of oscillator parameters and the convergence of theoretical $R(\lambda)$ model becomes very difficult.

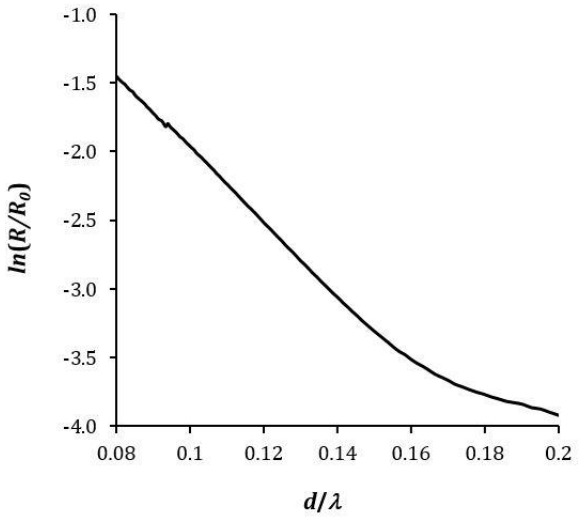

Fig. 3: *Development of the spectral reflectance with thickness of the SSCT layer.*

To overcome these numerical problems we splitted the SSCT layer on a system of 20 sublayers. Dielectric function of the *i-th* sublayer is in this approach modelled by the effective media approximation theory (EMA). For modelling of the dielectric function of 2D layers with large surface coverages the Maxwell Garnett (MG) EMA theory is often used [6, 9-10]. EMA model of Maxwell Garnett is a composition of a matrix medium *m* described by the dielectric function ε_m with inclusions *i* described by the dielectric function ε_i. Effective value of dielectric function ε_{eff} of composite media is in this model described by equation

$$\frac{\varepsilon_{eff}-\varepsilon_m}{\varepsilon_{eff}+2\varepsilon_m}=\delta_i\frac{\varepsilon_i-\varepsilon_m}{\varepsilon_i+2\varepsilon_m}\ , \tag{2}$$

where δ_i is the volume fraction of inclusions in the matrix medium. As the matrix medium we use Si and as the inclusion medium air. We gradually changed the volume fraction of inclusions in individual sublayers in correspondence with the requirement of increasing density of modelled SSCT layer. Resulting spectral reflectance $R\left(\lambda,d_{(k)},\varepsilon_{eff\,(k)}\right)$ based on the

MG EMA theory of dielectric functions with gradual volume fraction of inclusions in individual sublayers *k* of composite model is shown in Fig. 4.

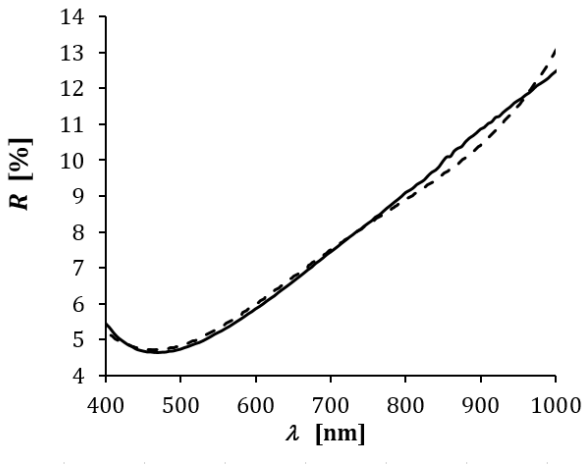

Fig. 4: *Spectral reflectance of the SSCT10 structure (line), and reflectance model for composition of 20 SSCT sublayers with gradient of dielectric function defined by MG EMA approximation (dashed).*

By using the MG EMA theory for description of dielectric function development in a multilayer system describing the nanostructured SSCT layers acceptable theoretical model of the spectral reflectance $R(\lambda)$ can be obtained. By using this approach in combination with the scattering matrix formalism the information about the volume fraction of voids development with the thickness of the SSCT layers can be obtained.

Acknowledgement

Author would like to thank Professor Kentaro Imamura and Professor Hikaru Kobayashi from the DFCM ISIR Osaka University, Japan, for cooperation in this research. The results were developed within the research projects supported by the Japan Society for the Promotion of Science and Osaka University research project „Analysis of Properties of the SSCT Layers“, Kobayashi Laboratories, ISIR, Osaka University, Japan. The work was supported by grant of Science and Technology Assistance Agency APVV-15-0152, Scientific Grant Agency VEGA 1/0676/17 and 1/0076/15, Centre of Excellence of Power Electronics Systems and Materials ITMS 26220120003, ITMS 26220120046, and project ITMS 26210120021.

References

[1] K. Imamura, F.C. Franco Jr., T. Matsumoto, H. Kobayashi: Ultralow reflectivity polycrystalline silicon surfaces formed by surface structure chemical transfer method. *Appl. Phys. Lett.* **103** (2013) 013110.

[2] K. Imamura, T. Nonaka, Y. Onitsuka, D. Irishika, H. Kobayashi: Light trapping of crystalline Si solar cells by use of nanocrystalline Si layer plus pyramidal texture. *Applied Surface Science* (2016), http://dx.doi.org/10.1016/j.apsusc.2016.04.132

[3] D. Irishika, K. Imamura, H. Kobayashi: *Sol. Energy Mat. Sol. Cells*, **141** (2015).

[4] K. Imamura, T. Nonaka, D. Irishika, H. Kobayashi: *ECSD Solid State Lett*., **4** (2015) Q63-Q65.
[5] S. Jurečka, T. Matsumoto, K. Imamura, H. Kobayashi: Multifractal analysis and optical properties of nanostructured silicon layers. *Applied Surface Science*, **395** (2017).
[6] S. Jurečka: Theoretical Model of the Physical System: Optimization by the Genetic Algorithm. In: Ioannis Dritsas: Stochastic Optimization - Seeing the Optimal for the Uncertain. InTech, Vienna (2011), ISBN 978-953-307-829-8.
[7] H. M. Branz, V. E. Yost, S. Ward, K. M. Jones, B. To, P. Stradins: Nanostructured black silicon and the optical reflectance of graded-density surfaces. *Appl.Phys. Lett*. **94**, (2009) 231121.
[8] L. Rosenfeld: Theory of Electrons, Dover Publications, New York (1965).
[9] J. C. Maxwell Garnett: *Philos. Trans. R. Soc. Lond*. A203, 385 (1904).
[10] T. C. Choy: Effective Medium Theory: Principles and Applications. Clarendon Press, Oxford (1999).