Scattering of roughened TCO films – modeling and measurement

Sven Schröder[1], Angela Duparré[1], Kevin Füchsel[1,2], Norbert Kaiser[1], Andreas Tünnermann[1,2], James E. Harvey[3]
1: Fraunhofer Institute for Applied Optics and Precision Engineering, Albert-Einstein-Straße 7, 07745 Jena, Germany
2: Friedrich-Schiller-University, Institute of Applied Physics, Max-Wien-Platz 1, 07743 Jena, Germany
3: University of Central Florida, College of Optics and Photonics / CREOL, 4000 Central Florida Boulevard, Orlando, FL 32816-2700, USA

sven.schroeder@iof.fraunhofer.de

Abstract: The scattering properties of transparent conductive oxide (TCO) films into dielectric and semiconductor surrounding media are modeled and compared to experiment. The new approach is not only valid for smooth optical films but also for films with enhanced roughness in order to generate light trapping structures for thin film solar cells.

OCIS codes: (310.0310) thin films, (350.6050) solar energy, (290.0290) scattering, (240.5770) optics at surfaces, roughness

1. Introduction

The scattering properties of thin film coatings are often seen as an unwanted effect caused by residual fabrication errors of the substrate or the intrinsic nanostructure of the film [1]. For certain applications, however, rough surface and interface structures may be used to tailor the light distribution for specific needs. Thin film solar cells are a promising alternative to conventional wafer-based solar cells with respect to material and fabrication costs. Yet, the rather small thickness of the active layer (~1 µm) requires effective coupling of the incident sunlight into the film (see Fig. 1). This can be achieved by using structured interfaces that lead to light trapping inside the active layer.

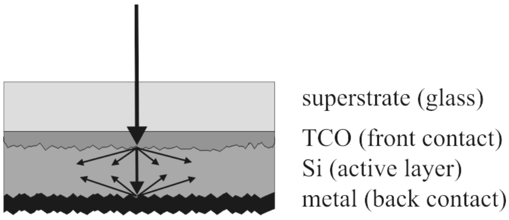


Fig. 1: Layer structure of a thin film solar cell with roughened interfaces to induce light trapping.

Appropriate scatter models are essential to predict the scattering distribution of a given interface structure and to define interface specifications in order to maximize the efficiency of thin film solar cells. Currently used procedures to optimize light trapping structures are:

- Trial and error: Thin film solar cells are processed with rather arbitrarily roughened interfaces. The effect of interface roughness is estimated after processing and testing of the complete solar cell.
- Approximate scattering theories: Although these theories provide a direct link between the interface roughness and the scattering properties, their application is confined to certain limiting cases: The classical Beckmann-Kirchhoff theory [2] contains a paraxial assumption that confines its applicability to small scattering angles. Scalar or vector perturbation theories, on the other hand, are only valid for very low roughness levels (compared to the wavelength of light) [3] and, consequently, low scattering efficiencies.
- Rigorous electromagnetic calculations: Although this approach offers exact solutions to the scattering problem, its practical application is often limited to simple regular, periodic structures [4]. Even if sufficient computational power for scatter simulations of stochastic surfaces is available, there still remain critical issues regarding the sampling of real topographies.

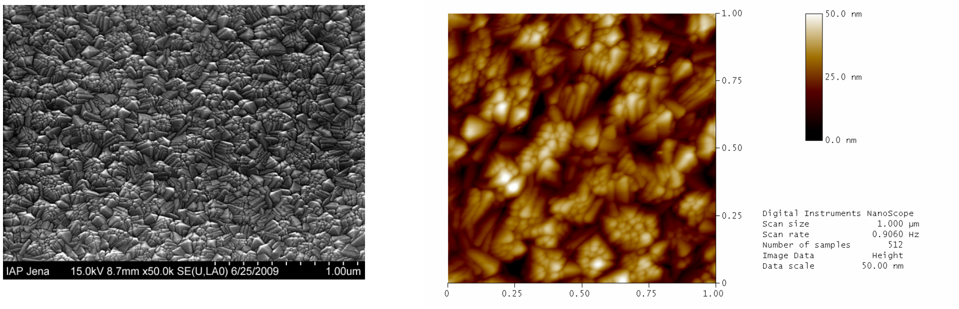
In general, modeling approaches that make use of the statistical properties of stochastic surfaces instead of relying on the knowledge of the exact topography have the advantage of inherent ensemble averaging. Recently, a new scattering theory, the Generalized Harvey-Shack (GHS) theory, has been developed which exhibits the advantages of both the vector perturbation theory and the classical Beckmann-Kirchhoff scattering theory with the limitations of neither [5]. The new approach should be valid for both optically smooth and rough surfaces. In particular, the intermediate case of moderately rough surfaces can not be treated satisfactory by existing theories.

2. Experimental

The final goal of this study is to model the scattering distribution of roughened TCO films into Si layers based on real surface topography data. This shall be accomplished using the following procedure:

(i) Fabrication of rough TCO coating on glass substrate: The challenge for this part is to deposit TCO films with considerable surface roughness but sufficient electrical properties.
(ii) Roughness analysis of TCO surface through Power Spectral Density (PSD) functions determined by Atomic Force Microscopy (AFM) and White Light Interferometry (WLI).
(iii) ARS measurement of TCO films
(iv) Modeling of the Angle Resolved Scattering (ARS) of the TCO/air interface
(v) Comparison of measurement and modeling results
(vi) Modeling of ARS of TCO/Si interface

i) TCO films were deposited onto glass (B270) superstrates using pulsed DC magnetron sputtering. The deposition process was adjusted such that the intrinsic thin film roughness was enhanced by maintaining the electrical properties required for the front contact film.

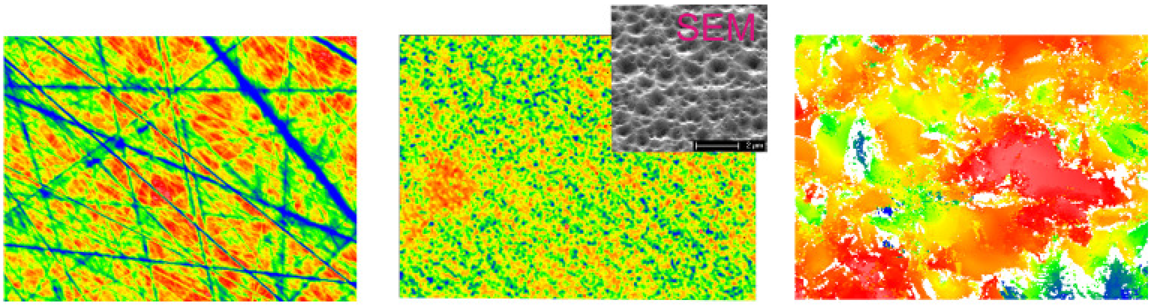


(a) (b)

Fig. 2: Interface structures of TCO films. (a) SEM image (field of view ca. 2x2 µm²), (b) AFM (1x1 µm²).

Since no sufficiently large diffuse scattering can be expected for the intrinsically rough TCO films, the interfaces were roughened using additional procedures such as sand blasting, lapping, and etching before or after coating.

ii) After thin film deposition and roughening, the surfaces were characterized using WLI and AFM as well as qualitatively using Scanning Electron Microscopy (SEM). Exemplary results of three TCO surfaces are shown in Fig. 3:



(a) (b) (c)

Fig. 3: WLI images (field of view 105x141 µm²) of roughened TCO films.
(a) lapped, rms roughness 5 nm, (b) chemically etched, rms roughness 24 nm, (c) sand blasted, rms roughness 2.5 µm.

From the surface topography data, Power Spectral Density functions (PSDs) and Autocovariance functions (ACF) are calculated as input for the scatter modeling procedure.

iii) Angle Resolved Scattering (ARS) is defined as the power ΔP_s scattered into the solid angle $\Delta\Omega_s$ normalized to $\Delta\Omega_s$ and to the incident power. For measurements in the forward scattering hemisphere with polar angles θ_s between 90° and 270°, ARS is equivalent to the Bidirectional Transmittance Distribution Function (BTDF) times cos θ_s.

ARS measurements were performed at 633 nm at normal incidence using the instrumentation described in [2]. The results are shown in Fig. 4.

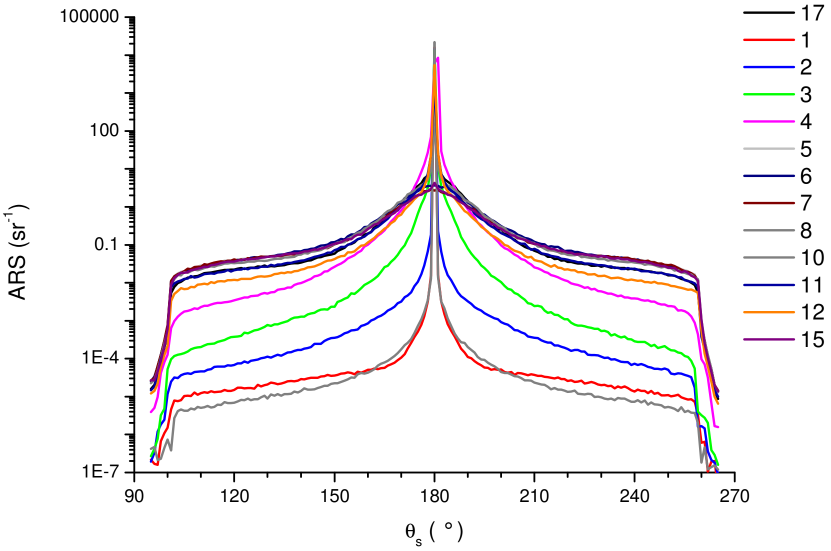


Fig. 4: ARS measurement results at 633 nm for different samples.

The experimental results clearly reveal a gradual transition from almost perfect specular reflection (peak at $\theta_s = 180°$) to diffuse scattering as the surface roughness increases (roughness values not shown).

iv-vi) For the scatter modeling, the GHS theory needs to be modified in order to calculate the scattering into the forward hemisphere. Once the ARS of the TCO surface into air as surrounding medium will be modeled in agreement with the measurement results (Fig. 3), the scattering distributions of the same structures into silicon can be predicted.

References

1. S. Schröder, A. Duparré, A. Tünnermann, "Roughness evolution and scatter losses of multilayers for 193 nm optics," Appl. Opt. 47, C88-C97 (2008)
2. P. Beckmann, A. Spizzichino, The Scattering of Electromagnetic Waves from Rough Surfaces, (Pergamon Press, New York, 1963)
3. J. M. Elson and J. M. Bennett, “Vector Scattering Theory,” Opt. Eng. 18, 116 (1979)
4. R. Dewan, D. Knipp, “Light trapping in thin-film silicon solar cells with integrated diffraction grating,” J. Appl. Phys. 106, 074901 (2009)
5. Harvey J. E., Krywonos A., Stover J. C., „Unified scatter model for rough surfaces at large incident and scatter angles,“ Proc. SPIE 6672, 66720C (2007)