Wide angle beam spectroscopic ellipsometer development and application for the investigation of solar cell technology ZnO layers

PhD thesis booklet

Csaba Ferenc Major

Supervisor: Dr. Miklós Fried

Hungarian Academy of Sciences, Research Institute for Technical Physics and Materials Science (MFA)

2009
Preface

Ellipsometry is a key optic measurement technique in today's thin layer research and in one of its leader industry, microelectronics. Development and production necessitates some methods of measurement to assist in control and feed-back tasks. Non-contact, non-destructive, fast and cheap measurement methods that do not require long sample preparation periods, are especially important. Ellipsometry, as is characteristic to optical measurement techniques, allows non-destructive investigations. A further advantage to other optical measurement methods is that it measures a complex refractive index, that is, it records phase information in addition to intensity differences. The method is absolutely sterile and, contrary to almost any other measuring and qualifying method, does not destruct slices and layers, therefore it is capable for in-line control during production. Due to this feature, ellipsometry is flourishing nowadays, moreover, biological and solar cell research-developement-technology applications are on the rise.
Analysis of the results from ellipsometric measurements is not a trivial task. Measurement data (complex refractive indices) are not in an obvious relation to the physical properties (layer thickness, refractive indices and chemical composition etc.) of the sample under investigation, therefore, they always have to be compared to the (hopefully less) idealised expected values of the optical model. Oftentimes, the construction and validation of these models are the key elements. Since they are obtained from very complex (including complex values) equations and functions, computational analysis methods are becoming emphasised and it is not by chance that the real development began after 1960, the time computers began to proliferate.

Ellipsometers available nowadays for sale are accurate enough for microelectronics and their rate is suitable for in situ or in-line measurements. A disadvantage of these instruments is that they only sample a single point. Point, in this case means a spot of some square millimeters (a tenth of a millimeter in the case of a focused beam), from which the instrument integrates information. Nowadays, we see a rise in big diameter wafer technology. However, mapping of some
square dm's of sample surface takes several minutes even for today's fast instruments, which precludes them from in situ mapping.

**Antecedents of the research**

Solar cell production is a competitive field of semi-conductor applications in Hungary, where various thin layer production techniques are fundamental. Utilisation of solar cells as a special and environment friendly energy source has a prospering tendency in satellite and space projects, as well as in earthly applications. As an effect of market conditions, enhancing productivity also has a growing role in technological development. Solar cells are built with larger and larger segment surfaces and the control of lateral homogeneity among various properties is implemented by traditional ellipsometers. Although there are mapping instruments as well, available polarizer sizes are still a limiting factor. In solar cell production we already have nearly 1 meter characteristic diagonals.

For the elimination of the problem, wide angle ellipsometry has been developed by Juhász György (MTA-MFA), Fried Miklós (MTA-MFA) and Horváth
Zoltán (SZFKI) as a method. The core of this method is that, in contrast to commercial ellipsometers, a non-parallel beam lights up a bigger surface of the sample. Optical arrangement allows that only sample-reflected, polarized light reaches the detector, which affects the accuracy of the measurement greatly. Each point of the detector can be mapped to a point of the sample, therefore, analysis of the measurement leads to a map with a given lateral resolution.

ZnO is an important material for solar cell research (too). The transparent/conductive features of ZnO (TCO, transparent conductive oxide) are utilised, therefore, it is important to qualify these properties in situ, or to investigate the inhomogeneity of the optical, electric and structural properties.

The research was conducted under the projects GVOP –3.1.1-2004-05-0435/3.0 AKF titled „Multispectral imaging refractometer” and NKFP 3/025/2001 titled „Solar cell technology innovation center”, in which I participated in 2005.
Objectives

The goal of my endeavours was to suggest a method for the enhancement of the simultaneously measurable measurement surface, to devise a variant of the equipment that is integrated for vacuum chambers, and a spectroscopic application. After the production of the prototypes of the different variants, I endured in calibration and real measurements to substantiate the proper workings of the equipments.

My aim was, moreover, to investigate ZnO (the transparent, conductive cover layer of photovoltaic layers), a very promising broad-band semi-conductor material of today. Investigations were aimed at the definition of the electronic properties of these thin layers by single ellipsometric measurements. Among the objectives, there was one, to substantiate the relationship between optical and electrical properties of the thin layers and the model parameters by a proper optical model.
Theses

1.a At first, I suggested an optical arrangement suitable for the lighting of a multi-colour wide angle ellipsometer. To this end, I designed a point-to-point optical mapping system that had two advantages. One is that it is capable of utilising small polarizers irrespectively of sample sizes. The other advantage is that the only limiting factor to the simultaneously measurable measurement surface is the strength of the light source, irrespectively of optic systems. I made a simulation of the expected lateral resolution. The equipment can be scaled appropriately, therefore, can be made capable for the simultaneous investigation of unlimited sample sizes. I have participated in the design of the mechanics of the equipment, in the calibration of the optics, and in the execution of calibrational and real measurements [1, 3, 4].

1.b I have shown that the above (1.a) mentioned multi-colour equipment can be integrated for vacuum chambers. I have modelled the necessary optical arrangement and the expected efficiency. Yielding to the
limits of mechanical necessities, I have made possible the investigation of large surface samples in vacuum chambers. I have participated in the mechanical design, construction and calibration. We have installed the equipment in the vacuum chamber of the Erlangen Fraunhofer Institute where we conducted measurements.

2. I was the first one to make a suggestion for a spectroscopic variant of the wide angle ellipsometer. To this end, I have developed the optics of the above (1.a) mentioned instrument. I have adjusted the lateral and spectral resolution to the chip size of the CCD camera. I have participated in the stages of mechanical design and construction. We made calibrational measurements with the equipment and, on the analysis of the data, I have shown that the measurements of the developed equipment are appropriate.[1, 4, 6]

3. I have shown that Al-doped ZnO samples with various physical properties (transmission, electric resistance) can be separated by sole ellipsometric
measurements, according to conductivity and transmission properties of the samples. I have conducted ellipsometric measurements then, on the analysis of the Cauchy dispersion function, I have shown that there is a relationship between the given physical properties and the characteristic fitting parameters [2, 6].

4. I have shown that a relationship can be traced between the electric resistance and transmission of Al-doped ZnO samples and the parameters of the model dielectric function suggested by Adachi. This way, I allowed the deployment of samples according to electric conductivity and transmission properties by quick, non-destructive measurements. I have shown that there is a relationship between the electric resistance of ZnO samples, the gap energy, and the amplitude of the discrete exciton. I was the first one to show the relationship between transmission properties and the amplitude of the continuum exciton [5, 7].
References:

[1] Wide angle beam ellipsometry for extremely large samples
C Major, G Juhasz, Z Horvath, O Polgar, M Fried, PSS (c), 5, 5, 1077-1080, 2008

[2] Spectroscopic ellipsometry study of transparent conductive ZnO layers for CIGS solar cell application

[3] Non-collimated beam ellipsometry

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[5] Optical and electrical characterization of aluminium doped ZnO layers

[6] Characterization of Al-doped ZnO layers by wide angle beam spectroscopic ellipsometry
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Other scientific publications:

Dielectric function of disorder in high-fluence helium-implanted silicon
P. Petrik, M. Fried, T. Lohner, N.Q. Khanh, P. Basa, O. Polgar, C. Major, J. Gyulai, F. Cayrel, D. Alquier, Nuclear
Utilisation of the results

In June of 2009, we are going to construct wide angle spectroscopic ellipsometers for the experimental vacuum chamber of the Toledo University (USA, Ohio). Re-designed spectroscopic versions will be made for the investigation of micromorph structures and ZnO layers.

We plan to construct a wide angle spectroscopic ellipsometer for the lock-chamber linking vacuum chambers in the Hungarian Academy of Sciences, Research Institute for Technical Physics and Materials Science for the investigation of solar cell technology ZnO and CIGS thin layers.