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Practical Determination of Optical Constants from Spectral Measurements

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Based on comprehensive knowledge in solid state physics, nanomaterials, and optical sensor technology, he authored more than 50 scientific publications with several topics and three books.

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Optische Schichtdickenmessung mit miniaturisierten Spektrometern
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1 Introductory Remarks

Optical constants are specific properties of condensed matter that allow to describe in a simple way the interaction of light or other electromagnetic radiation with matter. There is always a requirement for optical constants values for estimating colour, reflection, internal total reflection, refraction, scattering, phase shifting, multilayer properties, or thin film thickness.

In general, we can distinguish between the dielectric constant ε and the refractive index n and the extinction (or absorption) index κ as optical constants, although they are strongly related to each other. The generally complex *dielectric function* $\varepsilon(\omega) = \varepsilon_1(\omega)+i\cdot\varepsilon_2(\omega)$ with the imaginary unit $i=\sqrt{-1}$ is the physically relevant quantity for describing the interaction of light with matter, while for discussing propagation of light in and through media the generally complex *refractive index* $n+i\cdot\kappa$ is the more proper quantity.

The diversity of condensed matter with insulators, oxides, semiconductors, compound semiconductors, metals, and alloys calls for a huge amount on various optical constants even in different spectral regions. Therefore, there exist numerous works on the determination of optical constants with either tabulated data, graphical representation, or a parametrization of the data for a certain model.

The *Handbook of Optical Constants of Solids* [1], edited by Edward D. Palik, affords the most comprehensive database of the refractive index and absorption index of technically important and scientifically interesting dielectrics, semiconductors, and metals in three volumes. The online version of the *Handbook of Optical Constants of Solids* (a set of even five volumes) can be found on ScienceDirect.com. Beyond that, the database is supplemented by tutorial chapters covering the basics of dielectric theory and reviews of experimental techniques for each wavelength region and material. Although these tutorial chapters contain a huge amount of information, not all described experimental techniques are up-to-date or recently developed techniques are not contained. Another comprehensive sources of tabulated data are the *Handbook of Optics II* [2], the *CRC Handbook of Chemistry and Physics* [3], and particularly for semiconductors the book *Optical Constants of Crystalline and Amorphous Semiconductors: Numerical Data and Graphical Information* [4] by Sadao Adacho. A special reference for particularly thin films is the book *The Optical Constants of Bulk Materials and Films* by L. Ward [5]. It covers the theoretical background, experimental techniques, and results for a wide range of materials of thin films. Beyond that optical constants are published in further books and in numerous articles in several journals. Many of the data in these references are also available from several online databases, the most prominent being http://refractiveindex.info and www.luxpop.com. Also some suppliers of measurement equipment provide databases, e.g. Filmetrics Inc. at http://www.filmetrics.com/refractive-index-database.

With regard to this huge amount of information on optical constants and methods how to determine optical constants the question may arise why this booklet is necessary at all? The answer is that in many modern applications where optical constants are needed often there is a lack of knowledge about such data. They are either not contained in any collection or simple methods for a pretty fast determination are missing. This booklet has the aim to shorten this gap by introducing briefly in two simply accomplishable measuring methods -spectral reflectometry and spectral ellipsometry- and in available models for the parametrization of optical constants for determination of n and κ from the spectral measurements.

It begins with some few physical basics of light and the interaction of light with matter as well as information on the relationships among (complex) dielectric function and (complex) refractive index. Then, we introduce in physical models for the dielectric function and in empirical models mainly developed for the refractive index. The latter originate from the demand to have a model for the dispersion of the refractive index -this is the wavelength dependence of the refractive index- of those materials that are used in optical instruments like microscopes and telescopes. Also the specialty of the optical constants of composites of at least two nonmixable components is considered. The next chapter is dedicated to methods and techniques for the determination of optical constants. The focus is set to spectroscopic reflectometry and spectroscopic ellipsometry, as they can easily be applied mainly in the most interesting spectral range from the near ultraviolet to the near infrared. They always result in spectra of characteristic quantities that are determined by the optical constants. The task is then to retrieve the optical constants from these spectra. This task can only be solved using complex algorithms together with a parametrization of the optical constants. So we give finally some guidelines for the practical determination of optical constants from spectral reflectometry and ellipsometry in the last chapter.

To write this booklet required reading and valuating of many monographs and a still larger number of publications on this subject. The total amount of published work is too immense to consider them all here. Therefore, I hope to have included the most relevant up to date, and apologize for all the contributions not considered here.

Last but not least, I want to thank my family for their support and patience with me during writing this booklet.

Aldenhoven, 05.02.2018 Michael Quinten