Beginning to see the light

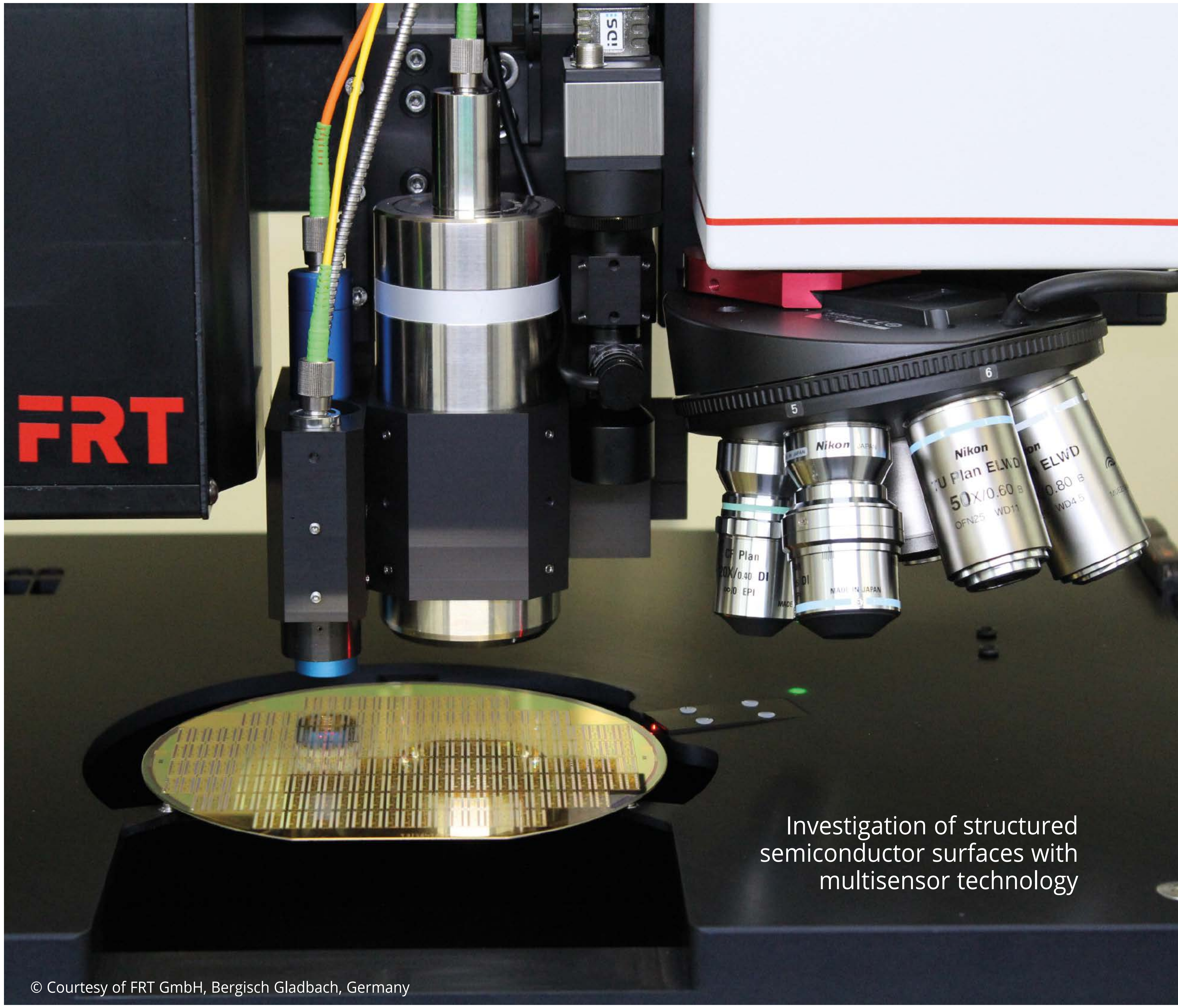
Calculating the reflectance of semiconductors with vias

Michael Quinten

The reflectance of a semiconductor wafer changes if vias or trenches are etched into the semiconductor. We present a rigorous far-field model that allows to calculate the reflectance under consideration of the geometrical properties of the via as well as possible transparent coatings on the wafer surface or transparent fillings in the via. For this the wafer is divided into units with a single via or trench. Each unit can further be divided into regions, the wafer surface region and the via or trench region. Transparent coatings or transparent fillings of the via are considered by simulating the reflectance of each region as the reflectance of a layer stack.

In smart electronics devices the basic semiconductor components must become smaller and more compact. This can be achieved by chip stacking in the manufacturing process. In this respect, etched vias and trenches establish vertical electrical connections (through-silicon vias, TSV) of upper-layer circuits and lower-layer circuits or shorter horizontal electrical connections (trenches) within a circuit.

For monitoring of the etching process and quality control of the vias and trenches the measurement of their critical dimensions (CD), i.e., their lengths, widths, diameters at top and bottom, the taper angles and their depths, is requested. The preferred measuring methods are optical methods since they are contactless and nondestructive. Among them the measurement of the reflectance of the textured surface and its interpretation with a proper model is a promising technique. We present a rigorous far-field modeling of broadband reflectance spectra of distinctly textured surfaces and apply it to semiconductor wafers with vias or trenches.



Investigation of structured semiconductor surfaces with multisensor technology

© Courtesy of FRT GmbH, Bergisch Gladbach, Germany

Basics of the model

For simplicity but without restriction of the generality, we consider in the following only vias with the shape of a truncated cone including perfect cylinders. Further, we consider the interference of the light reflected at the top surface and the light reflected at the bottom of the via. The detection spot (field-of-view) has the diameter D and the via opening has the diameter d_{top}. This corresponds to the situation of a reflectance measurement through a microscope with circular field-of-view as illustrated in Fig. 1. Cuboidic vias as well as rectangular field-of-views can also be calculated with similar results [1].

The basic idea of the current model is that the reflectance of each region can be simulated by the reflectance of a layer stack consisting of a substrate and a number N of thin layers with different thickness on the substrate. For $N = 0$ the stack consists only of the substrate. The reflectance (and transmittance) of a layer stack can exactly be calculated using either the Propagating Wave Model also called Abelès method [3, 4] or the r-t-φ model introduced first in the book of Azzam and Bashara [5]. For a survey on the calculation of the reflectance and transmittance of layer stacks we refer to [6].

The next step is to calculate the interference of the light reflected from region 0 and the light reflected from region 1. Then, the calculation of the energy flux density of the interference wave yields the reflectance R of the textured surface. It is

$$R = \left(1 - \frac{d_{top}^2}{D^2}\right)^2 \cdot R_0 + \left(\frac{d_{top}^2}{D^2}\right)^2 \cdot F^2 \cdot R_1 + 2 \cdot \left(1 - \frac{d_{top}^2}{D^2}\right) \cdot \frac{d_{top}^2}{D^2} \cdot F \cdot \sqrt{R_0 R_1} \cdot cos\left(\frac{2\pi}{\lambda} \cdot 2t\right).$$

with R_0 and R_1 being the reflectances of region 0 and 1.

As the bottom of the via (region 1) resides deeper than the wafer surface (region 0) by the depth t, the light coming out of the via has traveled the distance $2t$ before it can interfere with the light reflected at the wafer surface. Therefore, we have an extra phase factor $\exp(i \cdot 2\pi/(\lambda \cdot 2t))$ for the light reflected at the via bottom, leading to the cosine term in the reflectance.

Fig. 1 Sketch of a field-of-view with diameter D with cylindrical cavity with diameter d and depth t. Definition of the critical dimensions and the depth of a via with truncated cone geometry according to the SEMI norm [2]

Since the via forms only a part of the unit, the reflected light from region 1 can interfere only with a part of the light reflected in region 0. This is considered by the ratio of the via area to the area $\pi D^2/4$ of the field-of-view as a multiplier of the Fresnel coefficients of each region.

The factor F in the equation above considers several effects that diminish the amplitudes of the electromagnetic fields of the reflected wave in the via region. Two effects that are obvious from Fig. 1 are inclined walls and a curved surface. Both mainly lead to a decrease of the field amplitudes or the intensity due to multiple reflections at the via walls on the way downwards to the via bottom as well as upwards to the via opening. For silicon each reflection leads to a loss of intensity of 50 % averaged over s- and p-polarization and all angles of incidence. Finally, as the opening of a via is as small compared to the wavelength as diffraction becomes significant, diffraction must also be considered as source for losses of light coming out of the via region because the diffracted light will be reflected at the walls multiple times. Hence, the factor F can be assumed to consist of three factors: F_0 for the diffraction losses, F_1 for the losses due to inclined walls, and F_2 due to a curved surface. While F_1 and F_2 can be calculated to a certain degree (see [1]), F_0 can only be estimated. F_1 and F_2 are equal to 1 for a perfect cylindrical via but F_0 remains as a factor less than 1. A curved via bottom but to a certain extent also inclined walls can lead to beats in the spectral reflectance since the light gets not only reflected at the depth t but also at depths $t - \Delta t$ close to t.

Numerical examples

In this section we give selected numerical examples for the reflectance of silicon surfaces with perfect cylindrical vias. In all following examples we considered the spectral range from 250 nm to 1050 nm with a constant wavelength resolution of 0.5 nm. Diffraction and scattering are not considered, i.e., $F_0 = 1$. As the area ratio $ar = d_{top}^2/D^2$ has the most impact on the reflectance, we demonstrate the influence of ar on the reflectance spectrum for a via with $d_{top} = 5$ µm and depth $t = 5$ µm and for $ar = 0.5, 0.25, 0.125$, and 0.0625 in Fig. 2. For comparison, the upper and lower envelope are also drawn (red lines).

In the maxima of the cosine term we obtain $R_{si}(\lambda)$ as upper envelope. The lower envelope is given from the minima of the cosine and is $R_{si}(\lambda) \cdot (1 - 2\,ar)^2$. Obviously, the maximum modulation is obtained for $ar = 0.5$. This means that the maximum modulation is obtained if the diameter D of the field-of-view is $D = \sqrt{2} \cdot d_{top}$.

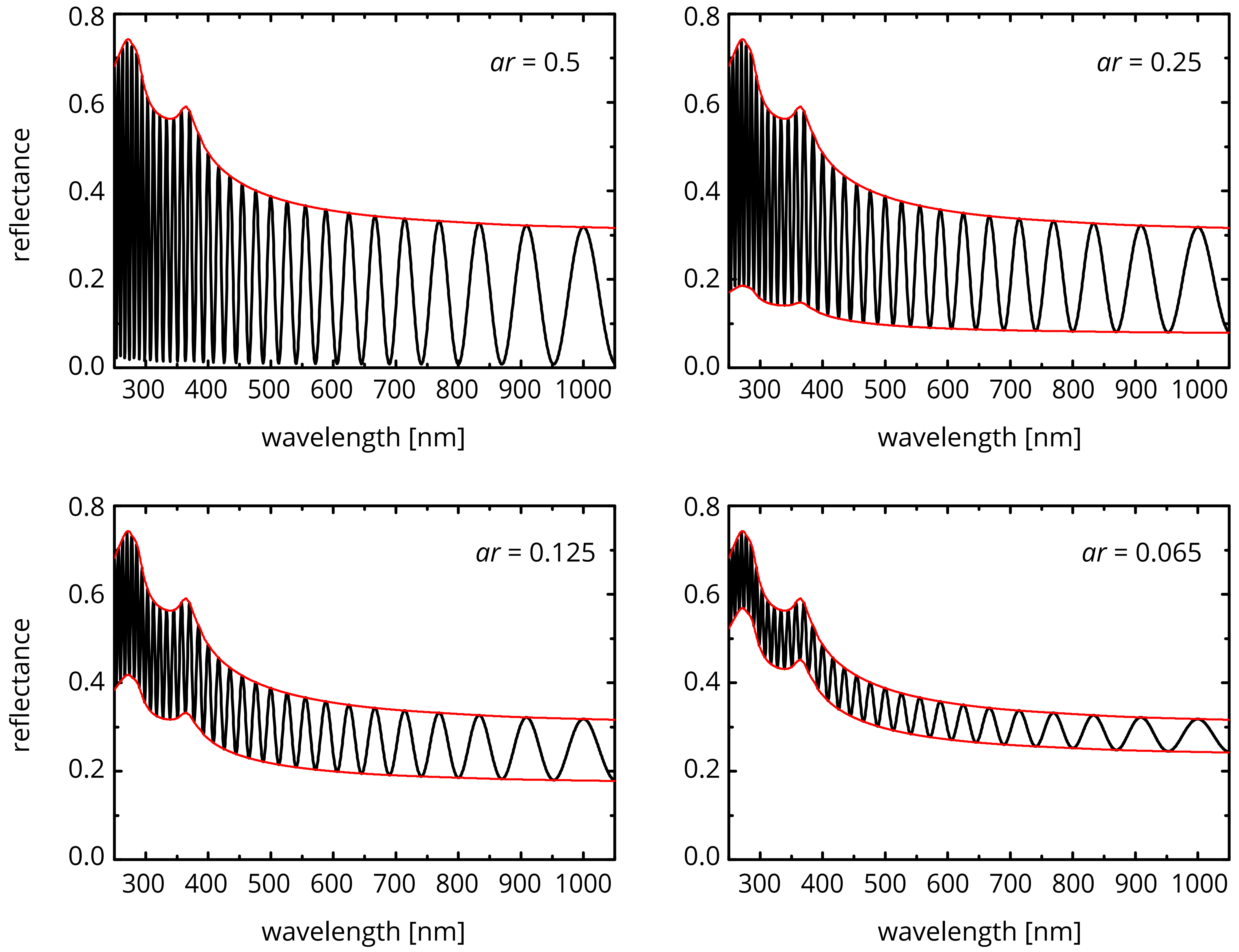


Fig. 2 Reflectance spectra for a silicon surface with perfect cylindrical via with d_{top} = 5 µm and depth t = 5 µm for varying ratio of via opening area to field-of-view area ar = 0.5 (largest modulation), 0.25, 0.125, and 0.0625. The upper and lower envelopes of the reflectance are also drawn

Michael Quinten

After his academic period from 1983 to 2000 Dr. habil. Michael Quinten joined ETA-Optik GmbH in 2001, Germany, where worked in research and development and as product manager for optical metrology. In 2007 he moved to FRT GmbH where he works in the optical sensor technology division as head of the R & D sensors department. In 1996 he founded Dr. Michael Quinten – Wissenschaftlich Technische Software where he develops and retails highly sophisticated scientific software.

Dr. rer. nat. habil. Michael Quinten,
Wissenschaftlich-technische Software,
52457 Aldenhoven,
Germany, phone: +49 2464 2649,
e-mail: ulmi.quinten@dn-connect.de

For inclined walls or a curved via bottom the reflectance spectra are quite similar to those in Fig. 2. The difference is caused by a factor $F < 1$, which leads to an upper envelope that is lower than $R_{si}(\lambda)$ and a larger lower envelope $R_{si}(\lambda)\cdot(1 - ar - F\cdot ar)$. Then, the modulation of the oscillation becomes still smaller than already caused by the area ratio *ar*. For examples we refer to [1].

The last examples are concerned with thin transparent layers on the top surface. Then, R_0 is different from R_1. Additional coatings of a silicon wafer particularly with silicon oxide (SiO_2) or silicon nitride (Si_3N_4) or even a double layer of these materials can often be found. These layers are intended as hard mask or buffer layer or were needed in the lithographic processing of the wafer. The thickness of these layers is in the order of a few 10 nm to a few 100 nm.

A thin film of a transparent coating changes the reflectance spectrum of the silicon wafer by introducing oscillations caused by white light interference at the interfaces of the thin film. The number of oscillations increases with increasing thickness, however for one complete oscillation the optical thickness $n\cdot d$ = refractive index × geometrical thickness must be at least ≈300 nm in the considered spectral range. For silicon wafers coated with such a transparent film and including a cylindrical via, the high-frequency oscillations due to the depth of the via superpose the low-frequency oscillations of the coatings. This is demonstrated in Fig. 3. The calculations are carried out for a perfect cylindrical via with d_{top} = 5 µm and depth t = 5 µm and for an area ratio ar = 0.25. The via bottom is uncoated. The via bottom is uncoated. The top surface is coated with 250 nm SiO_2 or with 150 nm Si_3N_4 or with the double layer of SiO_2 and Si_3N_4. For comparison, the reflectance spectra of the silicon surface coated with the thin films are also drawn (red lines).

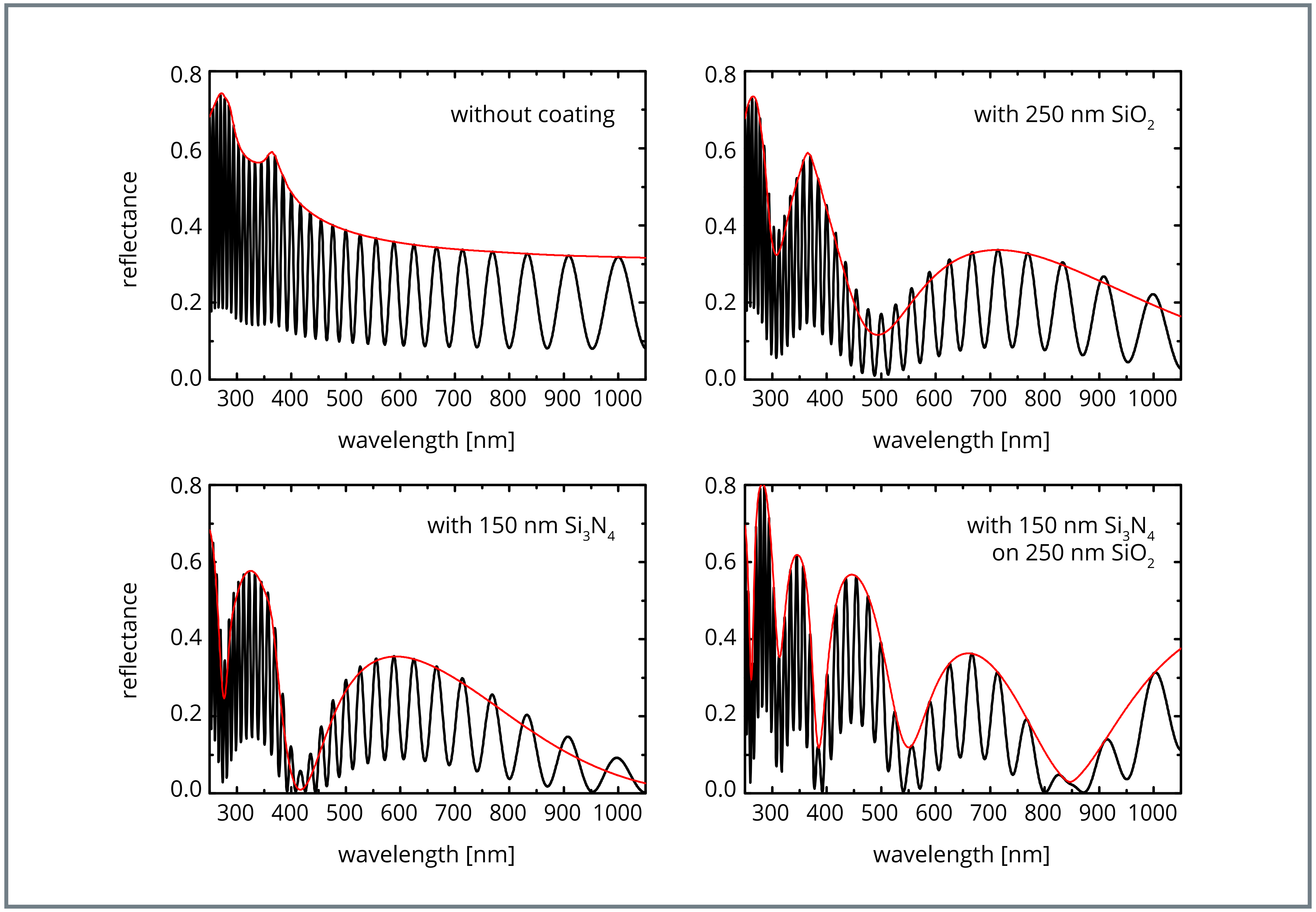


Fig. 3 Reflectance spectra of a silicon wafer with perfect cylindrical via. The top surface is coated with thin films of SiO_2 and Si_3N_4. The via has d_{top} = 5 µm and a depth t = 5 µm. The area ratio is ar = 0.25. For comparison, the reflectance spectra of the silicon surface coated with the thin films are also drawn (red lines)

One can recognize that the reflectance spectrum of the silicon wafer with coating is almost reproduced but is also clearly modified by the fast oscillations due to the via depth. A separation of both oscillations becomes difficult but not impossible.

Summary

The proposed rigorous model in the far-field is originally intended to be applied on semiconductor surfaces with vias to simulate broadband reflectance spectra of such structured surfaces. The main component of the model is the simulation of the reflectance of each region by the reflectance of a layer stack. By this way, we obtain a large variety of similar structured surfaces, since only thickness of the layers and their refractive indices are necessary to calculate the reflectance of each region. The effects caused by diffraction, scattering, inclined walls, or a curved via bottom are the same also for other materials.

The biggest advantage of the proposed far-field model compared to other techniques like rigorous coupled wave analysis (RCWA) or finite difference time domain (FDTD) is the computational efficiency. It does not need all the time-consuming elements like discretization of Maxwell's equations on a grid. Moreover, it can be combined with a least-square fit algorithm to determine critical dimensions and the depth of the vias and trenches.

The proposed model can be combined with an upstream fast Fourier transform to determine roughly the depth t of the via from a measured reflectance spectrum and then being used in a least square fit to determine the critical dimensions on top and on bottom, the curvature of the via bottom, and the via depth more precisely.

The most prominent restrictions of the proposed model are related to the via shape. As long as the deviations in shape can be considered to lead to a loss of intensity, they can be treated with this model via a factor similar to F_0, F_1, and F_2.

The proposed model is an optional part of a highly sophisticated software of the author for calculation and fit of layer stacks.

1. M. Quinten, Modeling of the reflectance of multilayered structured semiconductor surfaces, *Applied Physics A* 130, 620 (2024), https://doi.org/10.1007/s00339-024-07773-4
2. SEMI Draft Document 5410 – New Standard: Guide for Metrology Techniques to be Used inMeasurement of Geometrical Parameters of TSV's in 3DS-IC Structures
3. F. Abelès, *Ann. de Physique* 5, 596 (1950) and 706 (1950)
4. F. Abelès, *J. Phys. Radium* 11, 310 (1950)
5. R. M. A. Azzam, N. M. Bashara, Ellipsometry and Polarized Light, 2nd ed. (North-Holland, Amsterdam, 1987)
6. M. Quinten (2012), A Practical Guide to Optical Metrology for Thin Films, Wiley-VCH, Weinheim