Underlying theory

Outline

Introduction

UNIGIT is a universal grating solver that is based on two solving methods:

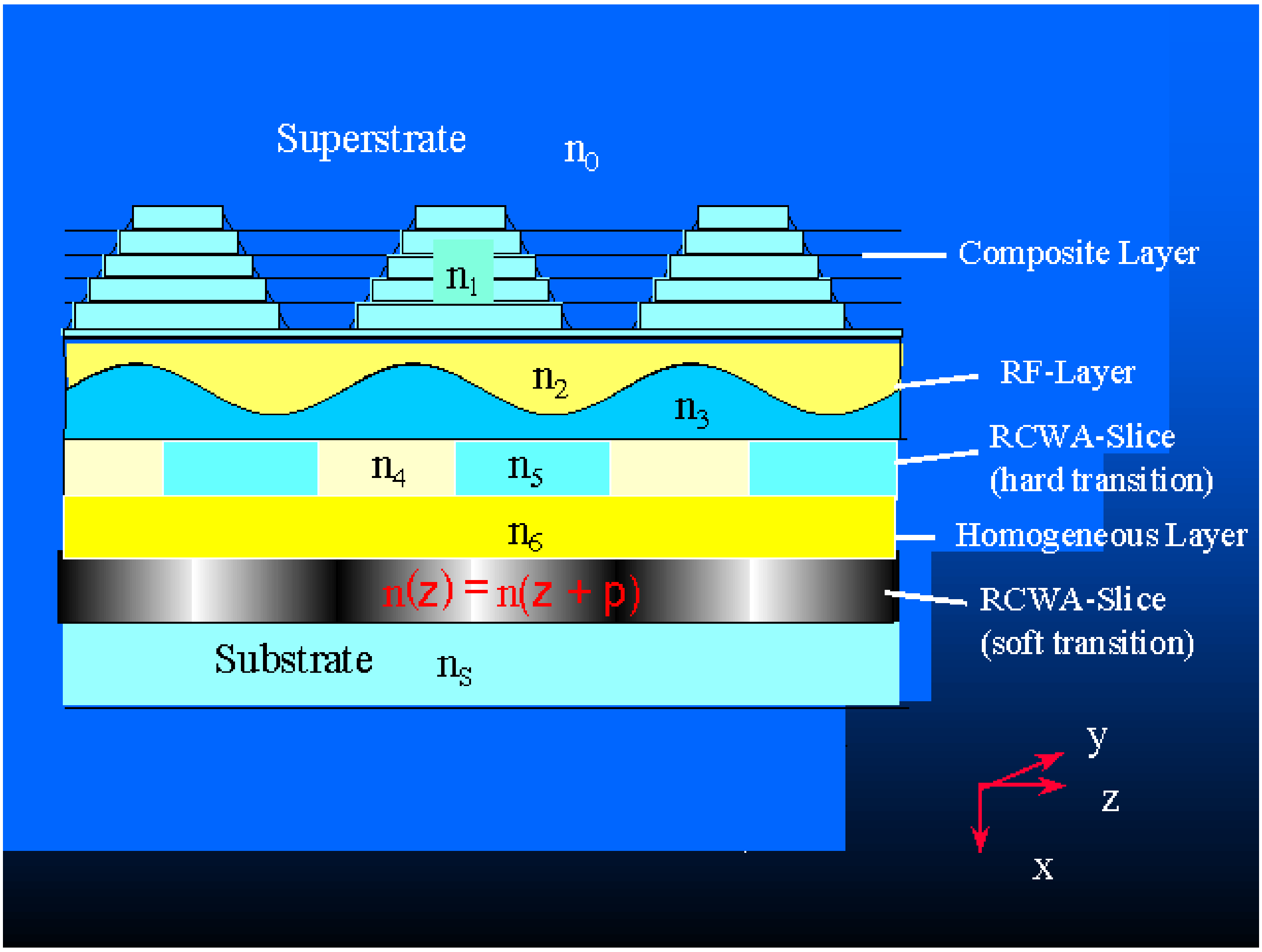
- the Rigorous Coupled Wave Approach (RCWA)
- the Rayleigh Fourier Method

In addition to that the solving methods are embedded in a matrix scheme. This matrix scheme permits the step-by-step solution of general layer stacks. A general layer stack can comprise different types of layers. These layer types are detailed below.

The Scattering Object

The basic composition of the scatterer corresponds to those known from an optical layer stack. In addition to an ordinary stack comprised by flat layers (multi-layer stack), the general stack may comprise layers with periodic patterns in one or two lateral directions.

A periodic change in one lateral direction is denoted as a grating or one-dimensional grating, respectively. Contrary, we call a scatterer having a periodicity in two lateral directions a crossed or a two-dimensional grating. The composite stack formed by flat as well as by patterned layers is called patterned multi-layer stack. The figure below shows a schematic example of a patterned multi-layer stack.



There are three basic types of elementary patterned layers:

- 1: layers with periodicity of the refraction index in one or two lateral directions,
- 2: layers with a periodic interface between two homogeneous materials,
- 3: homogeneous flat layers.

Associated, there are different solution methods for the different basic layer types:

- type 1: Rigorous Coupled Wave Approach (RCWA),
- type 2: Rayleigh-Fourier method,
- type 3: Classical Matrix Scheme - no coupling between the orders. in any case the outer borders of these elementary layers are flat.
- For the first layer type, the index variations may either be stepwise or gradually. Accordingly, the layers are called:
  - RCWA-layer with hard index transition, or
  - RCWA-layer with soft index transition.
- For layer type 2 there are two types of interfaces permitted:
  - Sinusoidal Interface
  - Polygonal Interface

Unfortunately, the Rayleigh-Fourier method is restricted to interfaces with a small aspect ratio. In the best case (sinusoidal interface and dielectric materials) it must not exceed 0.3. This limit has to be reduced correspondingly depending on the shape of the interface as well as on the material.

Here, the basic RCWA-layer offers a genuine mean to overcome these limitations. This can be done by the so-called slicing resulting in a stair-case approximation of the (arbitrary) interface to be treated. A sequence of RCWA-slices originating from such a slicing procedure are called a composite layer. The figure shows the slicing of a trapezoidal interface (top). In this way, all kinds of stacks can be treated correctly without any limitations.

There are no restrictions on the layer thickness. Basically, the full interference between the layers is assumed. The implementation of a thick homogeneous layer that compensates all interferences between above and below this layer is not yet implemented into the code. There are no restrictions concerning the number and the order of the different layers forming the stack.

The layer stack is embedded between two semi-infinite regions

- the superstrate
- and the substrate.

The superstrate is the medium above the layer stack from which the latter is illuminated. Generally, the superstrate will be air or vacuum. In case of immersion, other materials with refractive indices greater than one can be used. However, the superstrate must not have any absorption, i.e., the imaginary part of the refraction index must be equal to zero. If the detection takes place in the superstrate then one observes the reflected diffraction orders.

The substrate is below the layer stack. Usually, the stack is grown (and patterned) layer by layer onto the substrate. On the other hand, the substrate can also be air or vacuum. In any case, one speaks about transmission if the observation takes place in the substrate.

Both substrate and superstrate are characterised by the materials (see material editor) and by a certain thickness within these semi-infinite regions. If these thickness is set to zero, the diffractive powers in reflection or transmission, respectively, are calculated immediately at the interfaces between the stack and the superstrate/ substrate. Otherwise, by finite thicknesses, absorption losses can be taken into account for every diffraction order.

Apart from the superstrate, there are no restrictions about the materials of the layers.

Materials

Within the program, the optical properties are given by means of the complex refraction index. In this way, absorption and refraction are covered. Anisotropic behaviour is not included.

Basically, the material properties are input by means of the refraction index editor.

Here, the following options are implemented:

- Direct input of the refraction index: real part, imaginary part (in this option, dispersion is not taken into account.)
- Input from a data file and (if necessary) interpolation,
- Computation from various dispersion formulas.

Following dispersion formulas are available in the code:

Buchdahl

$$n = n_1 + B \cdot (n_2 + B \cdot n_3) \qquad k = 0$$

with:

$$A = 0.001 \cdot (\lambda - n_4) \qquad B = \frac{A}{(1 + 2.5 \cdot A)}$$

Cauchy

$$n = n_1 + \frac{n_2}{\lambda^2} + \frac{n_3}{\lambda^4} \qquad \mathbf{k = 0}$$

Drude

$$n = \sqrt{0.5 \cdot (A + B)} \qquad k = \sqrt{0.5 \cdot (A - B)}$$

with:

$$A = \sqrt{B^2 + C^2} \qquad B = n_1 - \lambda^2 \cdot \frac{n_3^2}{D}$$

and:

$$C = \lambda^3 \cdot \frac{n_3}{D} \qquad D = n_2^2 \cdot (\lambda^2 + n_3^2)$$

Lorentz

$$n = \sqrt{n_1 + k^2 + n_2 \cdot \lambda^2 \cdot \frac{A}{B}} \qquad k = \frac{0.5}{n} \cdot n_2 \cdot n_4 \cdot \frac{\lambda^3}{B}$$

with:

$$A = \lambda^2 - n_3^2 \qquad B = A^2 + n_4^2 \cdot \lambda^2$$

Sellmeier

$$n = \sqrt{1 + \frac{n_1}{1 + \frac{n_2}{\lambda^2}}} \qquad k = \frac{n_3}{n \cdot n_4 \cdot \lambda + \frac{n_5}{\lambda} + \frac{1}{\lambda^3}}$$

Square

$$n = n_1 + n_2 \cdot \lambda + n_3 \cdot \lambda^2 \qquad k = n_4 + n_5 \cdot \lambda + n_6 \cdot \lambda^2$$

Optical Excitation and Detection

Once the scatterer or patterned multi-layer stack is defined, the optical excitation and detection conditions have to be verified. Basically, the excitation or incidence comprises the angles of the incidence wave as well as the wavelength. On the other hand, one also wants to know where to put the detector in order to receive a certain diffraction order. Therefore, the detection conditions should be known.

Excitation

In general, the optical excitation originates from the superstrate. The incident light is considered to be a monochromatic plane wave impinging the layer stack under a certain polar angle in relation to the normal.

In order to fully characterize the diffraction the knowledge of the position of the incidence plane relative to the grating vector, i.e., the azimuthal angle of incidence is required.

From these value, the projection of wave vector into the layer plane can be computed. The wave vector is a conservation number for all homogeneous layers. It contains the well-known laws of classical layer optics, e.g., the coincidence of incident and outgoing plane and the validity of Fresnel's formulas.

However, the grating diffraction causes a cancellation of these laws, for arbitrary multiples of the reciprocal grating vector may be added to the wave vector depending on the diffraction order under consideration. (In 2D, the reciprocal grating vector is spanned in two not necessarily orthogonal directions.) Beside the specular directions in reflection and transmission, additional peaks occur called higher diffraction orders. If the polar angle θ and the azimuthal angle of incidence ϕ are given, the projections of the diffracted orders can be found uniquely. In case of an orthogonal (2D) grating, the projections to the first and second grating direction are given as:

$$\beta_1(m_1) = \beta_1(0) + m_1 \cdot \frac{\lambda}{p_1}$$

and

$$\beta_2(m_2) = \beta_2(0) + m_2 \cdot \frac{\lambda}{p_2}$$

The values are related to the wave vector 2 π / λ in vacuum. The mode indices mi may either be positive or negative integers. The larger the grating period di is getting, the denser the mode spectrum will be. The values mi = 0 correspond to the specular directions and are given via the angles of incidence by:

$$\beta_1(0) = n_0 \cdot \sin\theta_0 \cdot \cos\varphi_0$$

and

$$\beta_2(0) = n_0 \cdot \sin\theta_0 \cdot \sin\varphi_0$$

Here, n0 is the refraction index of the superstrate. Usually, this value should be a pure real.

If one intends to apply an absorbing superstrate (e.g., an absorbing immersion), then, the coupling into the superstrat has to be done via a prism. In any case, the components β will remain always real. To facilitate the handling, superstrate refractive indices n0 = 1 are permitted. Here, θ0 and ϕ0 mean the angles inside the superstrate.

Another essential issue is the polarization state of the incident light. As a matter of principle, UNIGIT always relates the polarization to the plane of incidence. Light with the vector of electric field strength oscillating perpendicular to this plane is called TE- or s-polarized. On the other hand, TM- or p-polarization means the coincidence of the vector with the plane of incidence. Since all computations are performed fully complex, i.e., amplitude (or efficiency) and phase are computed, from this all other polarization states may be derived by means of superposition.

Without giving a proof, it shall also be mentioned that the basic polarization states (TE and TM) decouple only for the particular case of an one-dimensional grating in the so-called classical mount, i.e., ϕ0 = 0. Contrary, the so-called conical mount ϕ 0 .ne. 0 results in polarization coupling even for a one-dimensional grating.

Detection

In similarity, the detection is also defined by the angles Θ and Φ. Reflexes can only be observed in certain planes given by:

$$\varphi_1(m_1, m_2) = \operatorname{atan}\left(\frac{\beta_2(m_2)}{\beta_1(m_1)}\right)$$

This holds for transmission as well as for reflection. However, the angle relative to the normal is different for reflection and transmission due to the different refraction indices of the substrate and the superstrate. This is quite analogous to the refraction at flat layers:

$$\theta_r(m_1, m_2) = \operatorname{asin} \frac{\sqrt{\beta_2(m_2)^2 + \beta_1(m_1)^2}}{n_0}$$

and

$$\theta_t(m_1, m_2) = \operatorname{asin} \frac{\sqrt{\beta_2(m_2)^2 + \beta_1(m_1)^2}}{n_t}$$

It can be easy seen, that the angles only make sense if the refractive indices are real and greater than the absolute value of

$$\beta(m_1, m_2) = \sqrt{\beta_1(m_1)^2 + \beta_2(m_2)^2}$$

Only in this case, the associated diffraction mode can be detected in the far field. Accordingly, the number of non propagating, i.e., evanescent modes is usually higher for reflection in air or vacuum compared with transmission into the substrate. The condition is that nt > n0 holds. For large λ / di ratios all higher diffraction orders can be evanescent. (This depends on the polar incidence angle too.) Then, only the zeroth order propagates. This kind of grating is called zero-order grating.

Of course, the polarization state is also defined relative to the detection plane. This plane is spanned by the layer normal and the vector β(m1 , m2) of the detected mode. Even in the conical mount of one-dimensional gratings, a polarization coupling occurs, that means both polarization states of a higher diffraction mode may be observed concurrently though the excitation was done only in one state.

References

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