

1. General Description

Unigit is a rigorous diffraction solver for 2D (1D periodic) or 3D (2D periodic) multilayer stacks (see figure 1). It runs on PC with Windows NT, Windows 2000 or Windows XP.

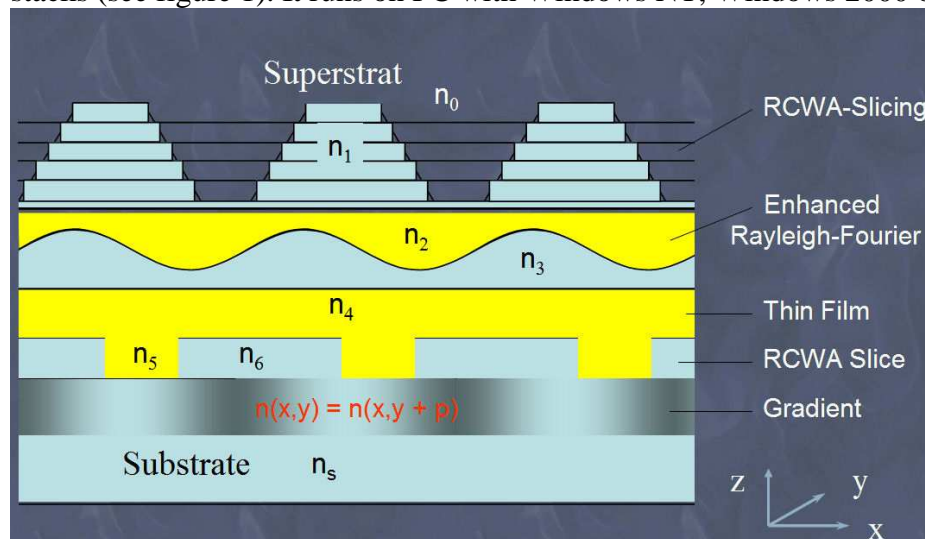


Figure 1: Schematic representation of a multilayer stack

Unigit comprises two basic solution algorithms:

- the Rigorous Coupled Wave Approach (RCWA) a.k.a. Modal Method with Fourier Expansion (see e.g., /1/, /2/ and /3/)
- and the Rayleigh Fourier Method (see e.g., /3/ and /4/) which is not rigorous).

Both algorithms are embedded in the same S-matrix algorithm (see e.g., /3/ and /5/) ensuring a high degree of stability as well as flexibility. The algorithms can be applied layer wise, i.e., one layer can be treated with Rayleigh-Fourier and another layer with RCWA.

The implementation was done in compliance with Lifeng Li's factorization rules (see e.g., /3/ and /6/).

The 2D algorithm follows closely Lifeng Li's paper /7/ as well as the descriptions in /3/. In addition, it offers the choice of the Lalanne method /8/ instead.

Unigit consists of a Graphical User Interface (GUI) and 3 computation kernels.

The computation kernels are:

- unigit_1D.exe: A solver for line/ space (1D) gratings in classical mount,
- unigit_co.exe: A solver for line/ space (1D) gratings in conical mount,
- unigit_2D.exe: A solver for non-orthogonal crossed (2D) gratings.

The 3 computation kernels can be utilized without the Unigit-GUI by embedding it in user applications. This can be done for example with Matlab, Visual Basic, C++ or C#.

2. Graphical User Interface

The GUI of Unigit is shown in figure 1. It enables the user an easy and straightforward control of all operations.

3. Special Features

Unigit offers a number of special features such as:

3.1 Specification of the complex refractive index by means of

- Direct input as complex number,
- Various Dispersion Formula,
- or wavelength dependent interpolation from a data file.

3.2 Various basic layer types for 1D

- Flat Homogeneous Layer (Thin Film)
- Rayleigh Fourier Polygonal Layer: piecewise linear interface solved with Rayleigh Fourier Method
- Rayleigh Fourier Sinus Layer: sinusoidal interface solved with Rayleigh Fourier Method
- RCWA Slice (Hard Transition): standard RCWA with arbitrary number of different n&k regions
- RCWA Slice (Soft Transition or Gradient): RCWA with processing a bitmap with n&k values
- Slicing Polygon: piecewise linear interface which is automatically sliced into RCWA layers
- Slicing Fourier: interface described by parametric Fourier sum presentation of x and y which is automatically sliced into RCWA
- Sequence of Layers: arbitrary number of layers defined before can be saved and reused as a layer sequence.
- The slicing is done automatically by means of a separate slicing routine which is a part of unigit. The sliced profile can be shown directly in the layer editor as figure 2 shows.

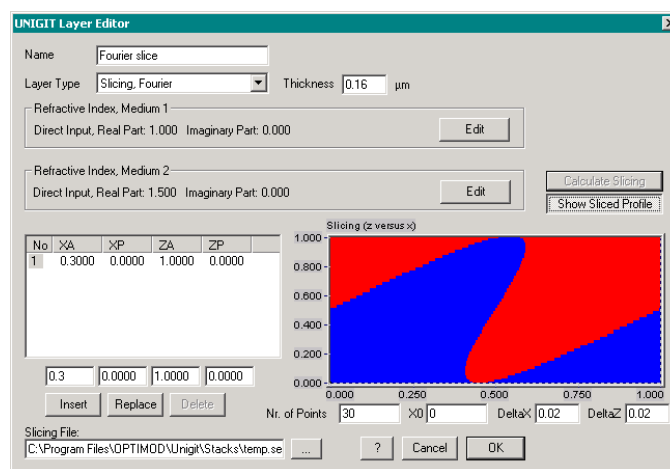


Figure 2: Sliced Fourier sum profile

3.3 Various Basic Layer Types for 2D Gratings

- Flat Homogeneous Layer (Thin Film)
- Rectangle-Patches Layer: arbitrary number of non-overlapping rectangles with arbitrary n&k defined at arbitrary position inside the 2D elementary cell.
- Ellipse Layer: one rotated ellipse with free ellipse power defined at arbitrary position inside the 2D elementary cell. The ellipse can be either related to the non-orthogonal axis of the elementary cell or to the global orthogonal x&y system. Figure 3 shows an example for an ellipse with power 4.
- Sequence layer for 2D similar to the 1D.

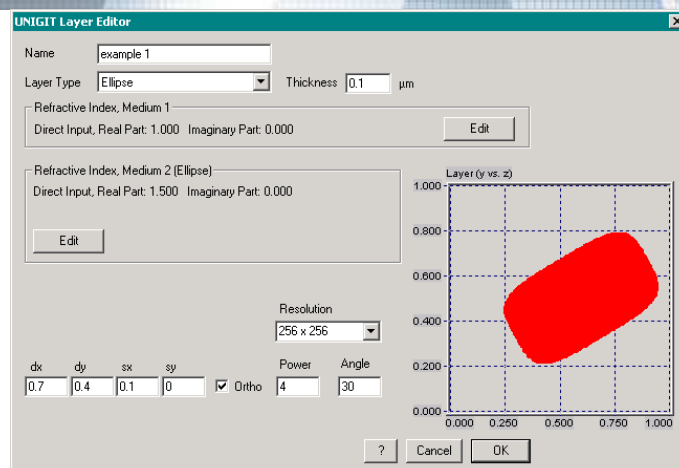


Fig. 3: Ellipse 2D layer (power =4, rotation angle = 30 deg)

3.4 Output and presentation of the results

Unigit provides the choice of calculating diffraction efficiencies, amplitudes, phases and ellipsometric parameters ($\cos\phi$ and $\tan\psi$) as a function of the wavelength, the incidence angle (θ or ϕ), the Rayleigh order or a free geometry parameter (saved as Ascii files). It also offers the option of plotting the results in a graphical window.

Moreover, the complete diffraction matrices in reflexion or transmission can be output as Ascii file for further processing.

References:

- /1/ M.G. Moharam, D.A. Pommet and E.B. Grann: "Stable implementation of the rigorous coupled wave analysis for surface-relief gratings: enhanced transmittance matrix approach", J. Opt. Soc. Am. A **12** (1995), pp. 1077-1086.
- /2/ Lifeng Li, "Multilayer modal method for diffraction gratings of arbitrary profile, depth, and permittivity," J. Opt. Soc. Am. A **10** (1993), pp. 2581-2591.
- /3/ J. Bischoff: „Beiträge zur theoretischen und experimentellen Untersuchung der Lichtbeugung an mikrostrukturierten Mehrschichtsystemen“, Habilitationsschrift TU Ilmenau, Germany, November 2000.
- /4/ D. Agassi and T.F. George, "Convergent schema for light scattering from an arbitrary deep metallic grating," Phys. Rev. B **33** (1986), pp. 2393-2400.
- /5/ Lifeng Li, "Formulation and comparison of two recursive matrix algorithms for modeling layered diffraction gratings," J. Opt. Soc. Am. A **13** (1996), pp. 1024-1035.
- /6/ Lifeng Li, "Use of Fourier series in the analysis of discontinuous periodic structures," J. Opt. Soc. Am. A **13** (1996), pp. 1870-1876.
- /7/ Lifeng Li, "New formulation of the Fourier Modal Method for crossed surface-relief gratings," J. Opt. Soc. Am. A **14** (1997), pp. 2758-2767.
- /8/ P. Lalanne, "Improved formulation of the coupled wave method for two-dimensional gratings," J. Opt. Soc. Am. A **14** (1997), pp. 1592-1598.