# Examples for UNIGIT Light

Along with the Demo Version of UNIGIT, some computation examples are provided. The objective is to show the user how to build a grating stack and how to run an application. To this end, the following stacks are prepared:

- **interface_1d.txt:** a plain interface between air (n = 1) and a dielectric material (n = 1.5),
- **arc_1d.txt:**   a plain interface with an anti-reflective coating,
- **dielgrat_1d.txt:** a dielectric grating (n = 1.5),
- **algrat_1d.txt:**   a metallic grating (Aluminum),
- **PR_BARC_1d.txt:**   a photo-resist grating on a Silicon substrate with a bottom anti-reflective coating (BARC),
- **two_layer_1d.txt:**   a double layer Chromium grating on a dielectric interface.

In the following, it will be briefly explained how to run these examples. (The online help may give you assistance if necessary.)

1. Plain Interface

After starting UNIGIT select the input file **interface_1d.txt** by means of the SELECT button of the STACK group. (The name of the stack file is then shown under ACTIVE STACK FILE.) Check the radio button Theta_i in the LOOP group to run a loop over the angle of incidence (AOI) and insert a start and a stop value as well as a step width (0; 89; 1 – meaning run from 0 through 89 degrees in step of one). Insert a wavelength value in the corresponding field (don't care much – the refraction index is fixed) and insert the truncation order from .. to.. (0; 0). Then verify the output conditions by clicking the EDIT button in the OUTPUT group (Select: Single Files; New File; Efficiency; Output Orders from 0 to 0, Check Reflection). Define the location where to write the result file under SAVE RESULTS IN and start the computation. After the computation is finished, you can view the results by clicking the ADD button in the RESULT FILE(S) group and selecting the corresponding reflection files with the extension *.re and *.rm for TE (s) and TM (p) polarization, correspondingly. The result should look similar to that shown in figure 1. You can easily see the 4% reflection for both polarizations at normal incidence and the Brewster angle at about 56 degrees. Of course you can choose a finer angular grid to find the zero in TM at 56.31 degrees.

Diffraction Efficiency
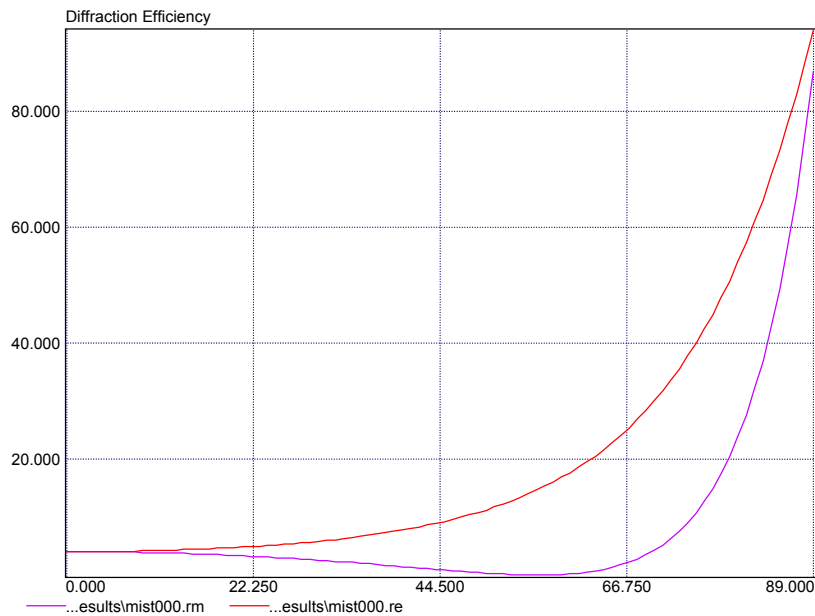
2. Anti-Reflective Coating

Select the input file **arc_1d.txt** and check the radio button Lambda in the LOOP group to run a loop over the wavelength and insert a start and a stop value as well as a step width (0.4; 0.7; 0.02 – meaning run the wavelength from 400 nm through 700 nm in step of 20 nm). Insert a 0 for the AOI and insert the truncation order from .. to.. (0; 0). Then verify the output conditions by clicking the EDIT button in the OUTPUT group (Select: Single Files; New File; Efficiency; Output Orders from 0 to 0, Check Transmission). Define the location where to write the result file under SAVE RESULTS IN and start the computation. After the computation is finished, you can view the results by clicking the ADD button in the RESULT FILE(S) group and selecting the corresponding transmission files with the extension .te and .tm for TE (s) and TM (p) polarization, correspondingly. The result should look similar to that shown in figure 2. Obviously, the transmission is 100 % at 500 nm. (The AR layer was optimized for $\lambda = 500$ nm and normal incidence according to $n = sqrt(n_1*n_2)$ and $h = \lambda/(4*n)$.)

Diffraction Efficiency
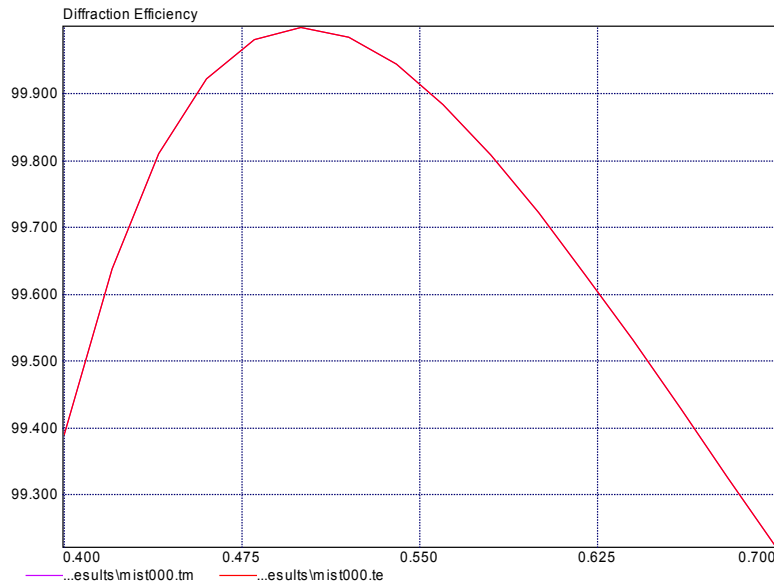
3. Dielectric Grating

This example is the first "real" grating to try. It is made from non-dispersive material with n = 1.5. It has a period of 0.3 microns, and equal lines/ spaces 400 nm in height. Select the input file **diel_grat_1d.txt.** Then enter 0.5 microns for the wavelength. Until, the truncation could be easily chosen to be 0 for plain interfaces. For a grating, the convergence strongly depends on the truncation number, i.e., where the modal expansion of the electro-magnetic fields is truncated for the sake of numerical calculation. Therefore, it is recommended to run firstly a convergence loop. To this end, check the radio button Truncation in the LOOP group and insert the Rayleigh orders that are kept in the computation (1;20;1 meaning from ±1 through ±20 in step of 1). After running the computation, the result files should look similar to that presented in table 1.

Truncation	TE	TM	Truncation	TE	TM
1	15.798	24.333	11	20.025	21.411
2	20.421	20.129	12	20.025	21.407
3	20.257	21.623	13	20.026	21.412
4	20.015	21.246	14	20.026	21.41
5	20.031	21.428	15	20.026	21.413
6	20.018	21.361	16	20.026	21.411
7	20.024	21.411	17	20.026	21.414
8	20.022	21.39	18	20.026	21.413
9	20.025	21.41	19	20.027	21.414
10	20.024	21.401	20	20.027	21.413

Depending on the required accuracy, a truncation between 4 and 9 seems to be appropriate. Now, you are probably interested in the diffractive behaviour of this grating. To this end check the radio button Theta_i in the LOOP group and insert (0; 60; 1) and change the grating period to 0.3 microns (use the stack editor). Check both Transmission and Reflection for the output file and choose output orders minimum = -1 and maximum = 0. From the results you will see that:

- the minus first order in reflection occurs at AOI > 41.8 degrees,
- the minus first order in transmission appears at AOI > 9.6 degrees,
- the total energy in all propagation orders (reflection and transmission) is 100 % (energy criterion).

4. Metallic Grating

Now, we shall consider a metallic grating. Select the input file **al_grat_1d.txt.** It is made from Aluminum, has a period of 0.5 microns and equal lines/ spaces being 200 nm in height. Again, you should first run a convergence test. Check the TRUNCATION button, enter (1;40;1) to specify the truncation loop and 0.7 for the wavelength. Your convergence curves (reflection) should look like those of figure 3. In spite of the improved models implemented in UNIGIT, the TM-convergence (pink curve) for metallic gratings is sometimes worse compared to TE.

Diffraction Efficiency

The next recommendation is again a loop over the AOI (0;50,1) with a truncation setting of 25. The resulting reflection curves for the 0. and –1. order are shown in figure 4. Clearly, a sharp change in the zeroth orders can be observed when the first orders start to propagate at AOI = 23.57 degrees.
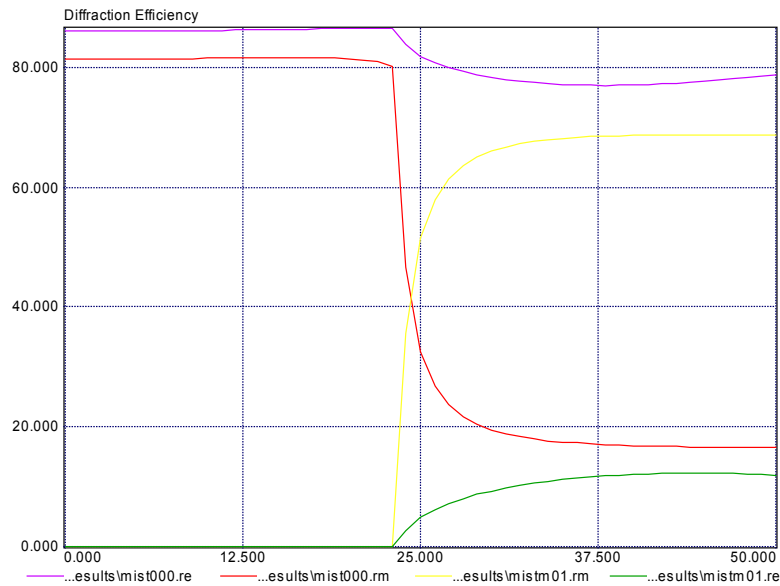
The resulting two stack files describe:

- PR_BARC_1D: A patterned photo-resist above a BARC layer on a Silicon substrate. The grating period is 0.5 microns. The PR-lines are 300 nm high and have a linewidth of 250 nm. The 100 nm thick BARC layer is not patterned.
- Two_layer_1D: A patterned Chromium double layer on a dielectric substrate. The grating pitch is 0.5 microns. The geometry is depicted in figure 5. This example gives a hint how to assemble non-binary gratings from rectangular slices. An automated slicing tool is available in the full version of UNIGIT.