A new user-friendly tool for simulating the efficiency of (multilayer) gratings

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Introduction

- Many x-ray facilities now use multilayer gratings in plane-grating monochromators (PGMs) as they provide high efficiencies in the tender x-ray range

- While there are lots of proprietary programs for simulating multilayer gratings, most of these have been designed for scientific applications in the UV-Vis-IR range and can be expensive

- For single-layer gratings, many researchers use REFLEC

  Schäfers and Krumrey, *BESSY Technical Report* 201/96 (1996)

- However, it is not possible to script REFLEC simulations, making its use rather laborious, especially when using it to design new (single-layer) gratings

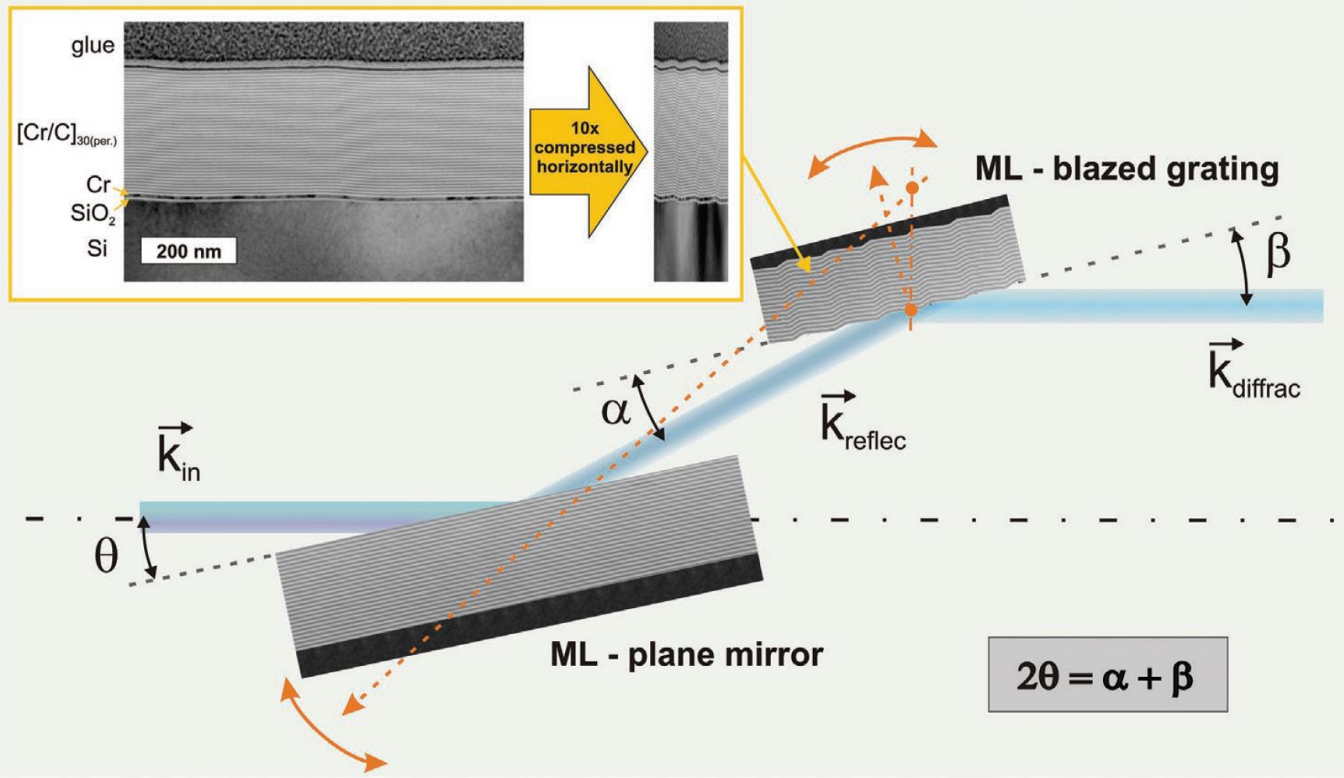
- Here we present alternative MATLAB software that we have developed based on GD-Calc, a freely available software tool for diffraction grating simulation

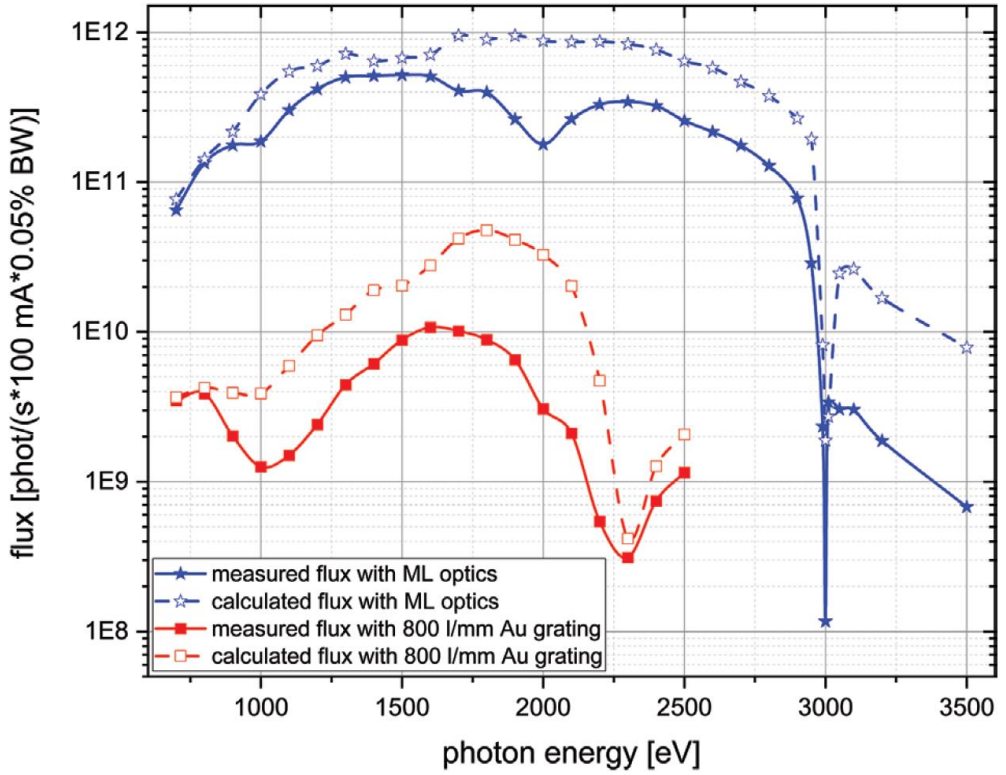
  Johnson, *Grating Diffraction Calculator (GD-Calc ®)* (2022) https://doi.org/10.24433/CO.7479617.v5

- Our MATLAB software enables the grating efficiencies of both single-layer and multilayer gratings to be simulated, ***and*** allows simulations to be scripted

diamond

Recent multilayer grating results (as reported on Tuesday!)





Werner et al., *Small Methods* **7**, 2201382 (2023)

The photon flux is increased by between 10× or 100× depending on the photon energy!

The first multilayer grating at Diamond!

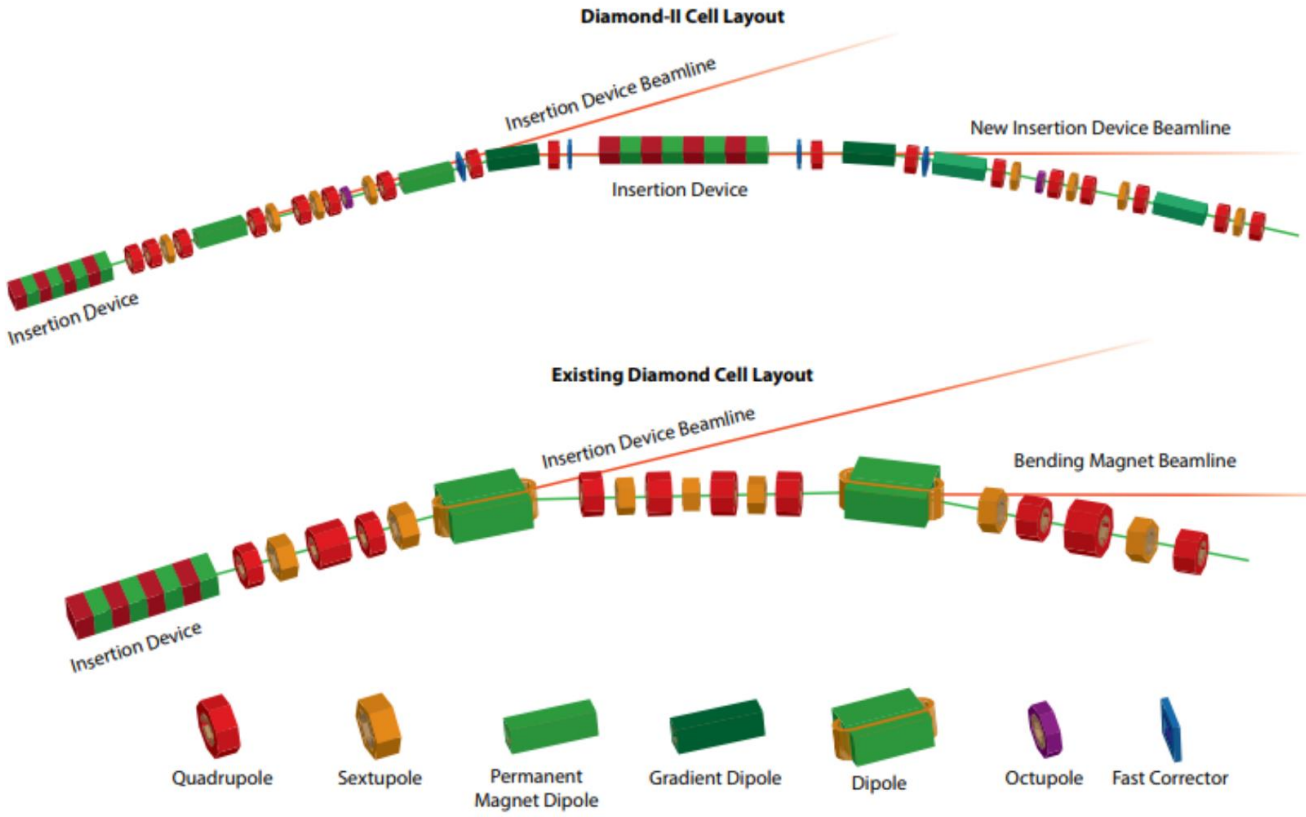
- Until recently our group's work on multilayer gratings has been solely theoretical

  Yang et al., *J. Synchrotron Radiat.* **24**, 168-174 (2017)

- A spherical variable line-spacing (VLS) grating for the I21 RIXS spectrometer has been coated with three multilayer stripes by Qiushi Huang's group (Tongji University)

- Stripe 1 was deposited in 2021, and the I21 beamline subsequently demonstrated a ≈ 30× increase in efficiency at the Ru L-edge at 2838 eV

The future of multilayer gratings at Diamond



- Many Diamond beamlines would benefit from higher grating efficiencies in the tender x-ray range (especially B07, B24, I08 and I21)
- Just over a week ago (5th September) the UK government officially confirmed the funding for the Diamond-II project

  https://www.diamond.ac.uk/Diamond-II.html
- One of the flagship beamlines for Diamond-II (I17 CSXID) will operate up to 3500 eV using a plane-grating monochromator, and therefore would benefit hugely from multilayer gratings

Optics fabrication capabilities at Diamond

- Diamond is in the process of significantly extending its in-house capabilities for fabricating optics
- An ion-beam figuring system is being commissioned (see Arindam Majhi's poster)
- A new multilayer deposition system will be delivered in October. This system will be able to deposit multilayer coating onto optics up to 1 metre long

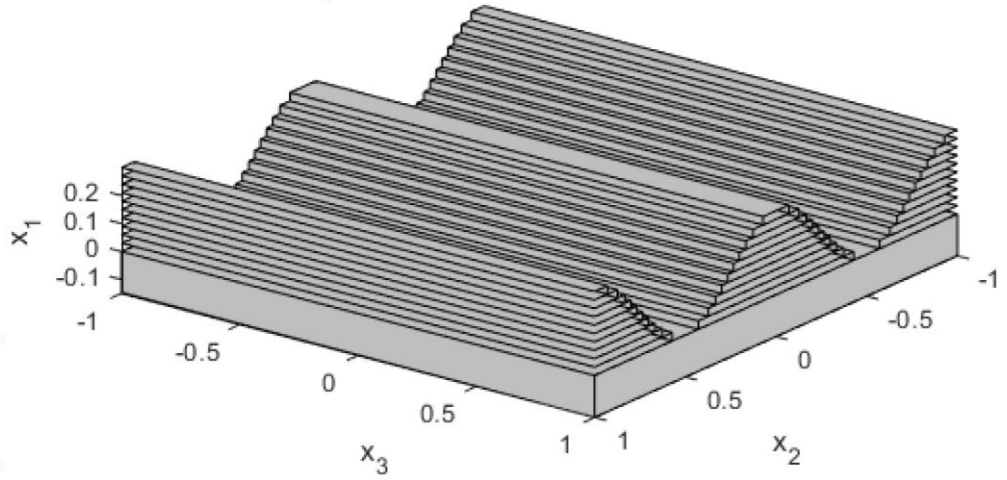
Which grating simulation software should we use?

- There are many options available, both commercial (e.g. RSoft DiffractMOD, UNIGIT, PCGrate, GSolver) and freely available (PPML, RawDog, RETICOLO etc.)

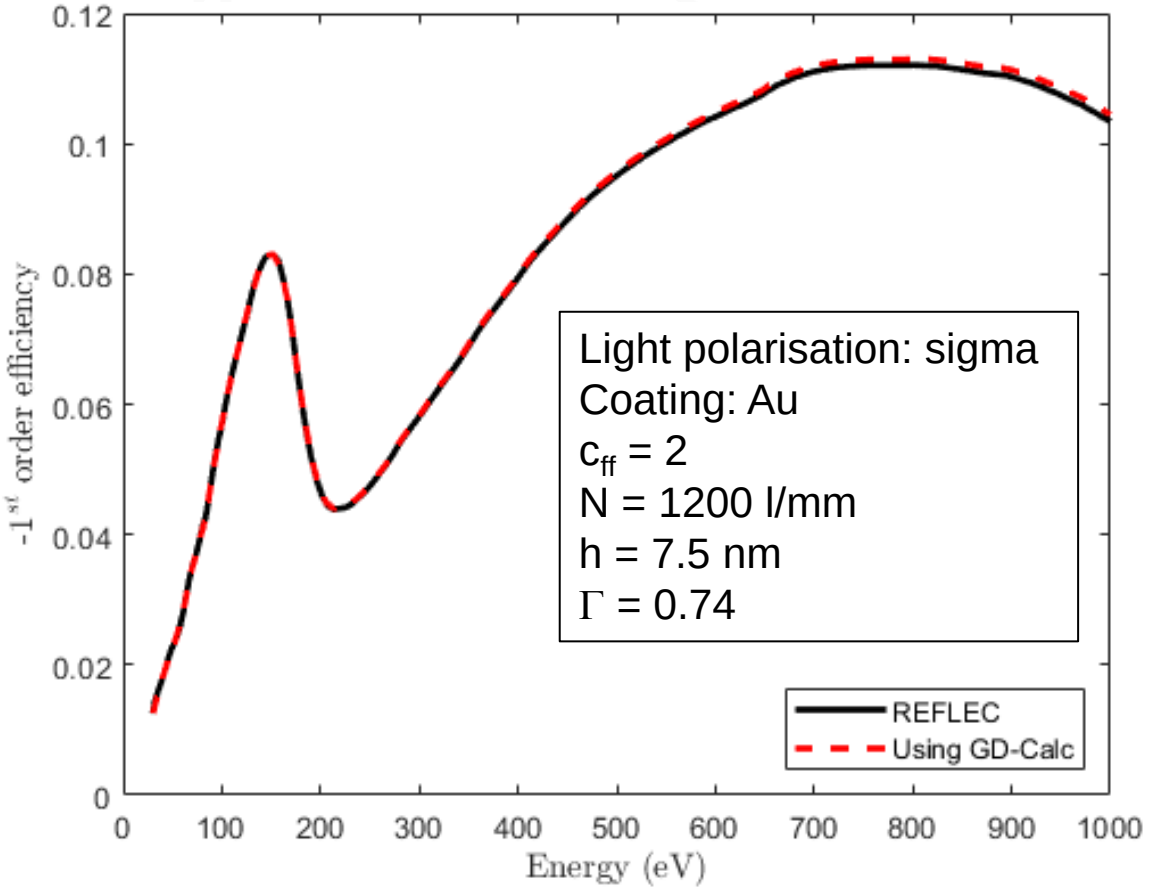
- We chose to work with GD-Calc, as it has been recently updated and has been used for various recent scientific publications (although not for synchrotron applications). The code uses the Rigorous Coupled-Wave Analysis (RCWA) method

Johnson, *Grating Diffraction Calculator (GD-Calc ®)* (2022)
https://doi.org/10.24433/CO.7479617.v5

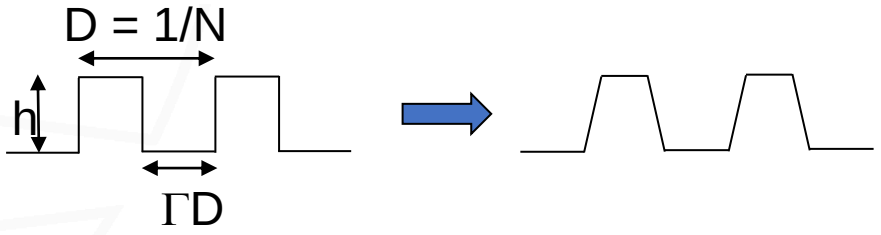
- In GD-Calc, gratings are described as combinations of rectangular blocks. This means that in principle it is more suited to simulating laminar gratings rather than blazed gratings



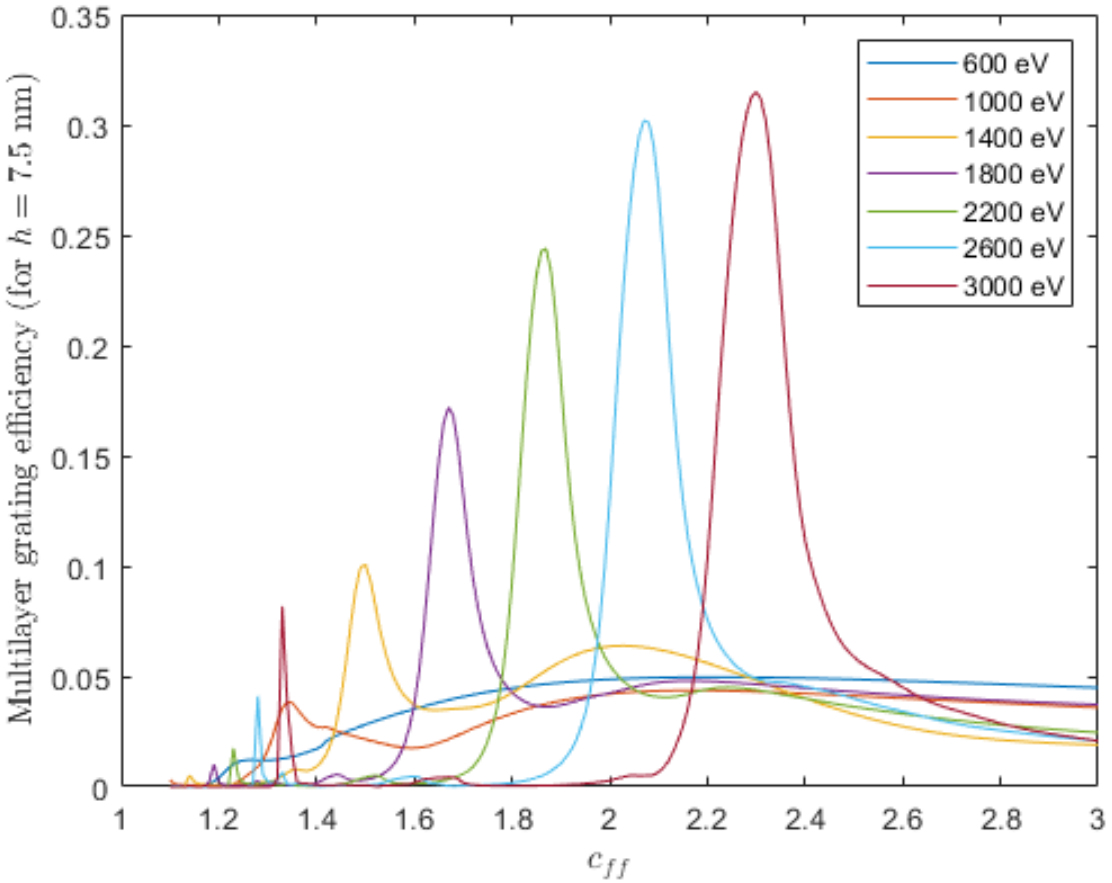
First steps: simulating a laminar grating

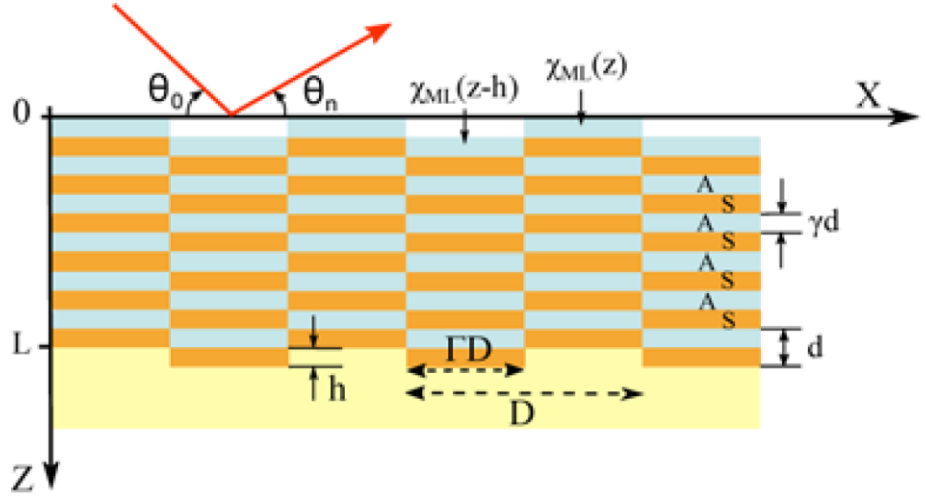


- We find good consistency between REFLEC (black) and using GD-Calc (red) for this simple case
- The code has not yet been extended to account for the more realistic trapezoidal profile where the groove walls are not vertical, but this should be a trivial improvement (using a staircase approximation)
- The effect of interfacial roughness is not included

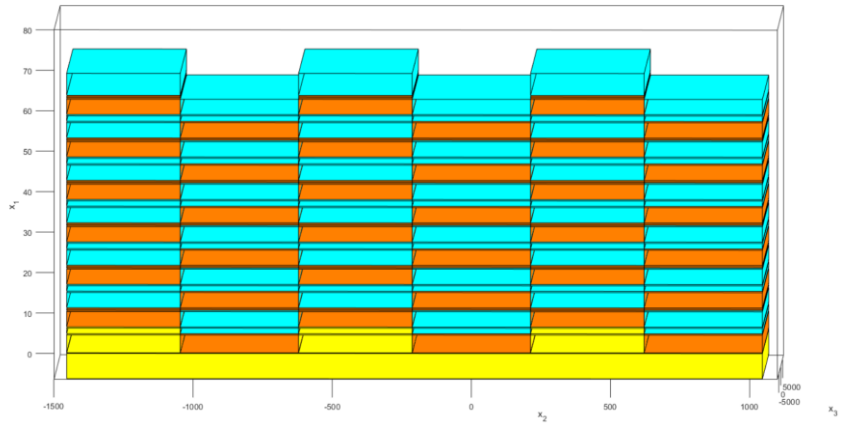


An example: a multilayer laminar grating for B07 (1)





Yang et al., *Optics Express* **25** 15987-16001 (2017)

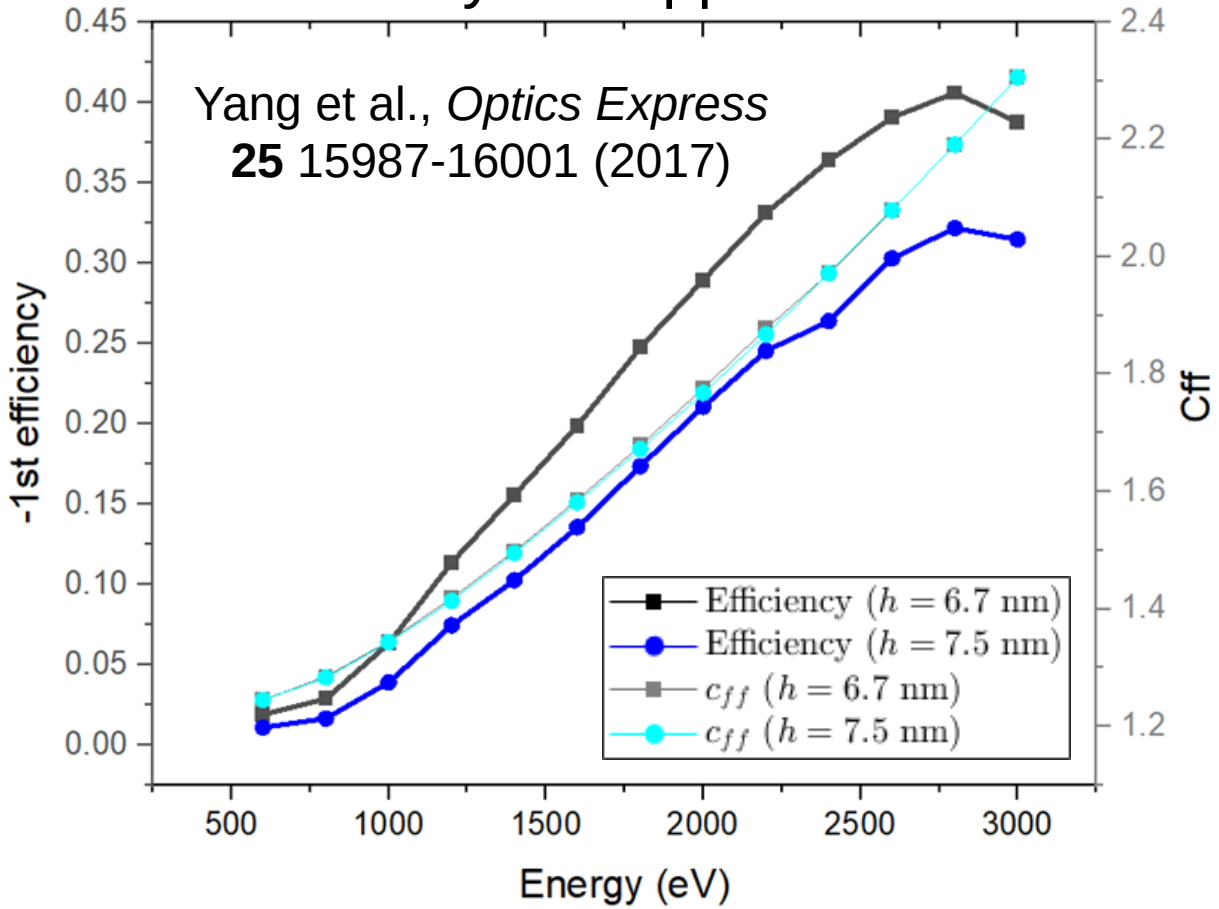


Here we have used our software to simulate the multilayer grating efficiency as a function of PGM c_{ff} at several photon energies

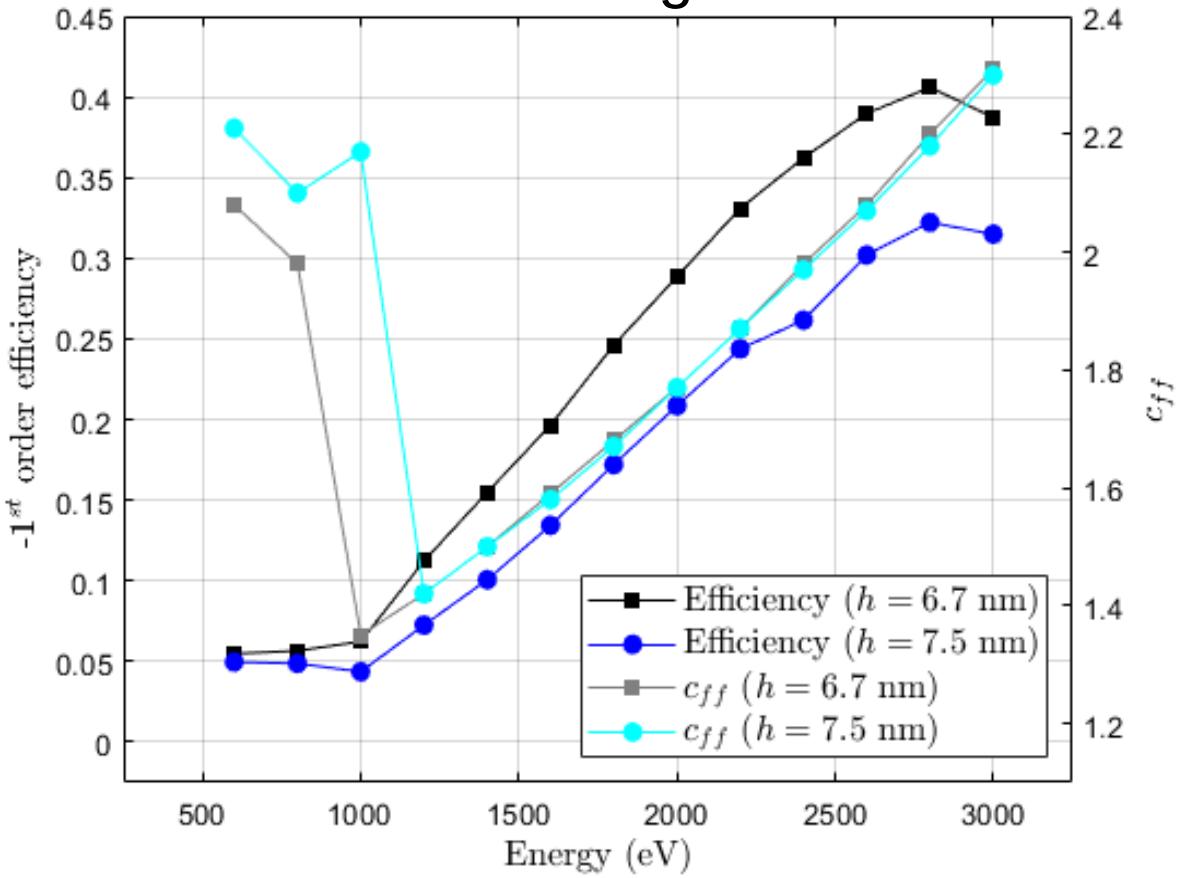
$$c_{ff} = \frac{\sin\theta_0}{\sin\theta_{n=1}}$$

An example: a multilayer laminar grating for B07 (2)

Analytical approach

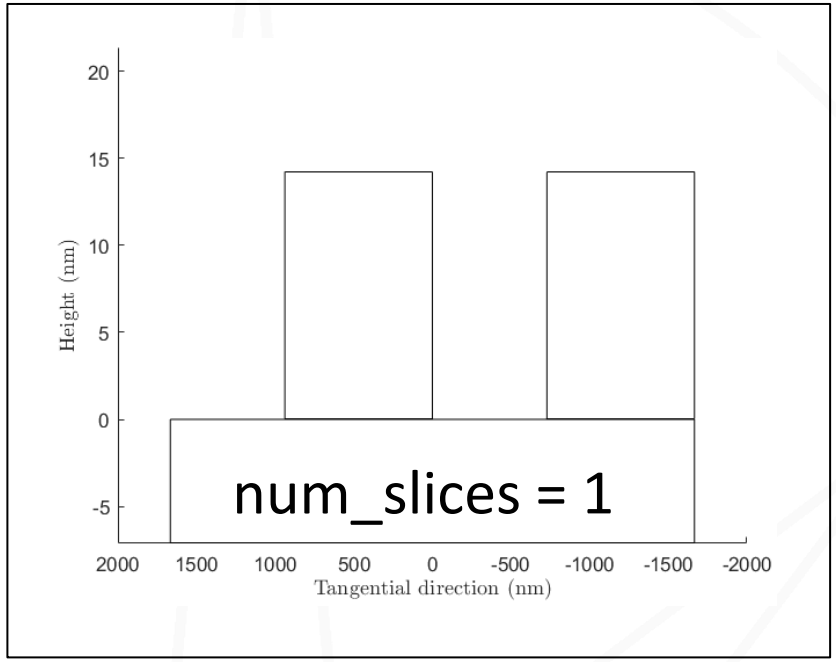


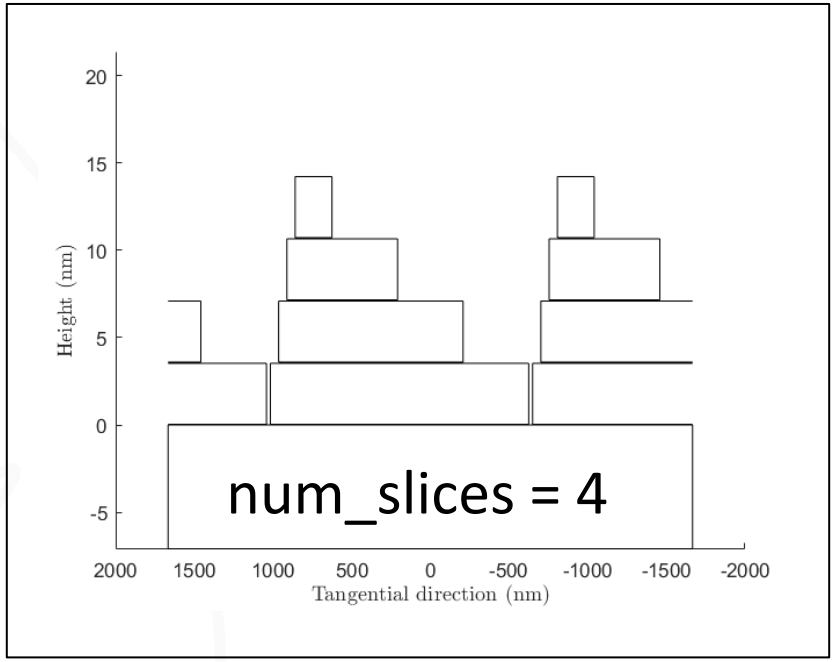
Our results using GD-Calc

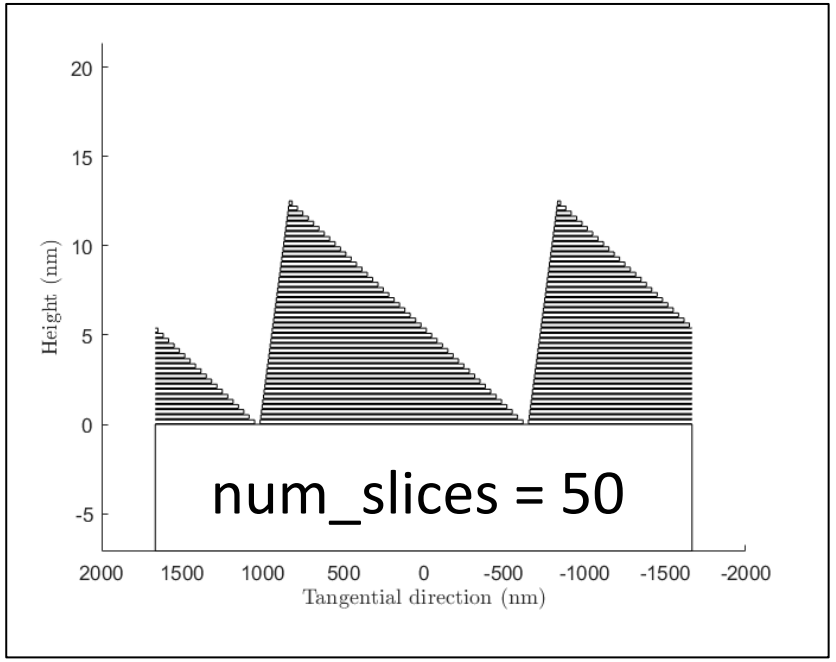


- Excellent agreement at high *E*
- At low *E* the ‘multilayer’ grating provides a higher efficiency if operated as a single-layer grating

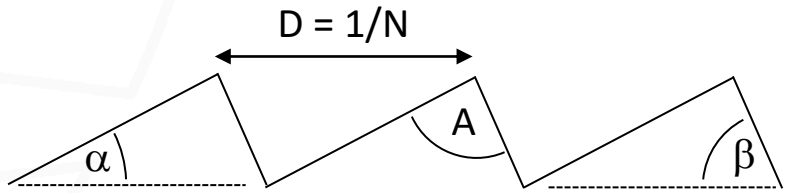
Using the staircase approximation for blazed gratings



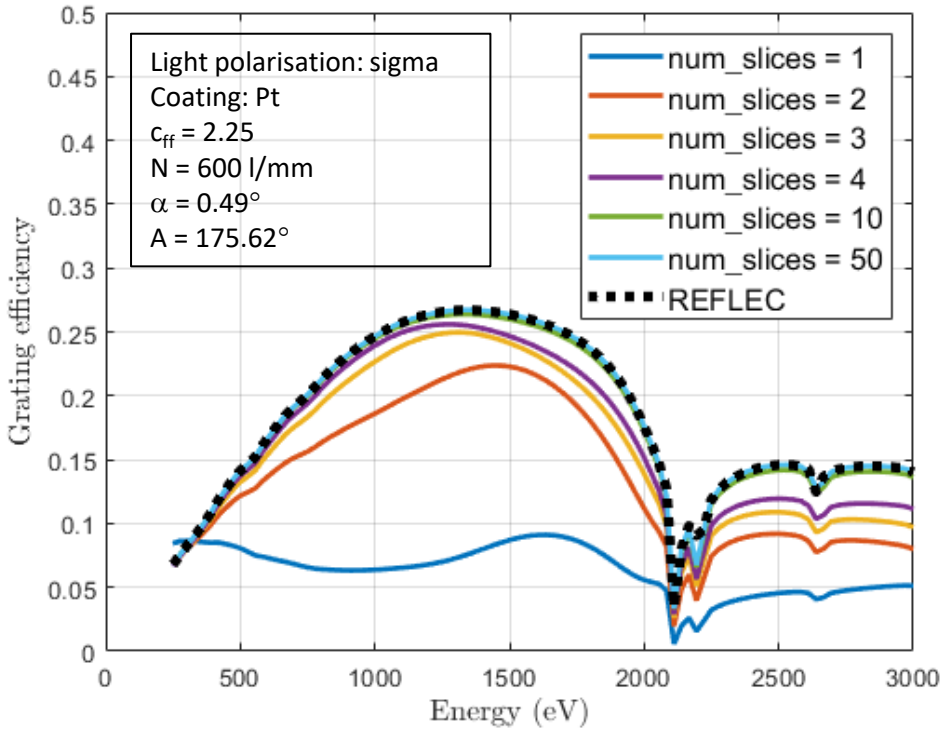


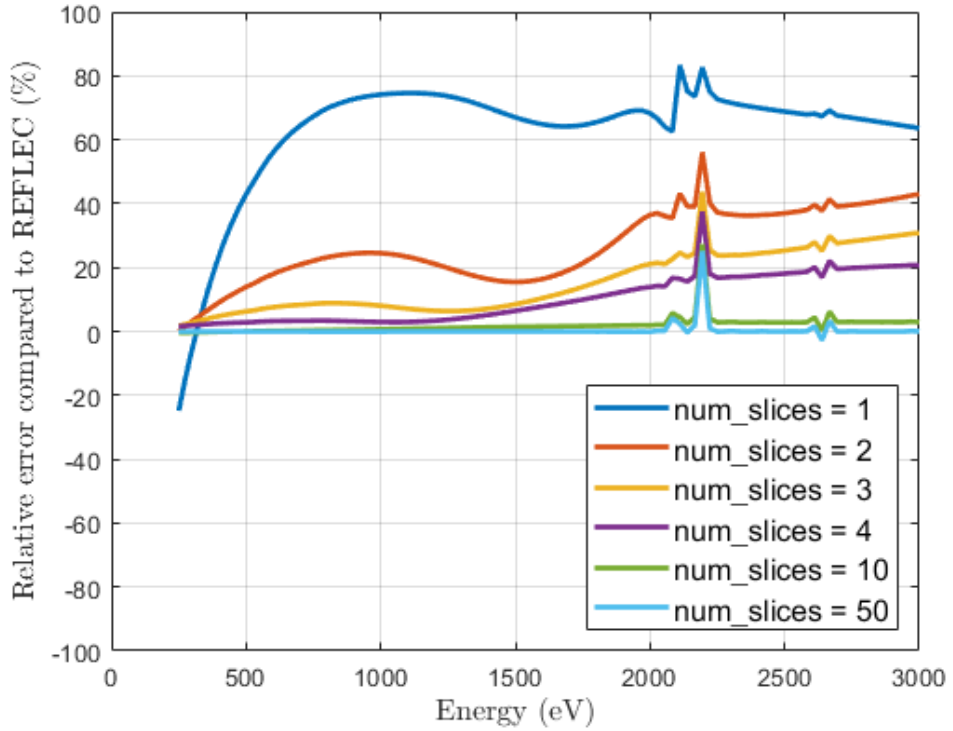


- A 1 slice approximation to a blazed grating is a laminar grating (of course!)
- In general, the higher the number of slices, the more accurate the simulation is likely to be

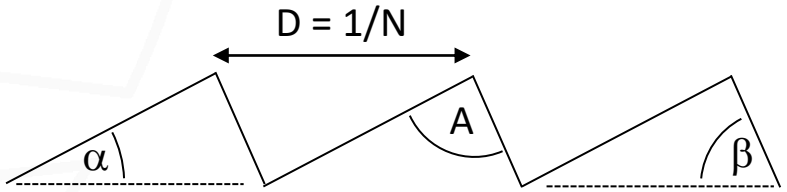


Simulating a blazed grating





- Simulation error (compared to REFLEC) is below 10% over most of the energy range when num_slices ≥ 6
- With num_slices = 10, the error is below 4% over most of the energy range



Time taken for simulating blazed gratings

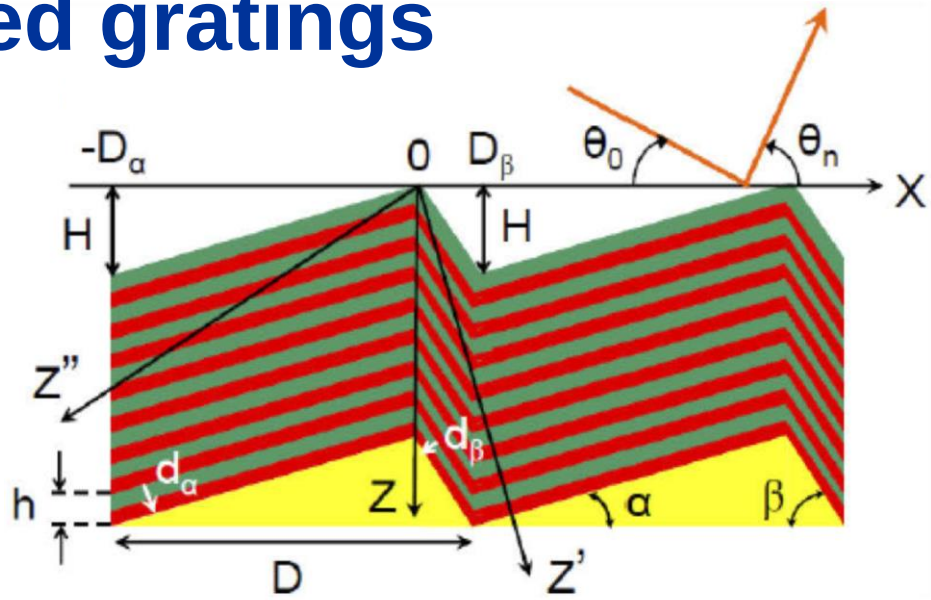
Software	num_slices	Number of energies	Time (s)
REFLEC	N/A	100	**~ 28**
GD-Calc	1	100	5.0
GD-Calc	4	100	8.0
GD-Calc	10	100	15.0
GD-Calc	20	100	**27.4**
GD-Calc	50	100	62.4

- For this grating, if GD-Calc is operated with num_slices = 20, the time taken for the simulation is comparable
- With this number of slices, the relative error compared to REFLEC is < 0.2% (apart from near to the absorption features in the Pt optical constants)

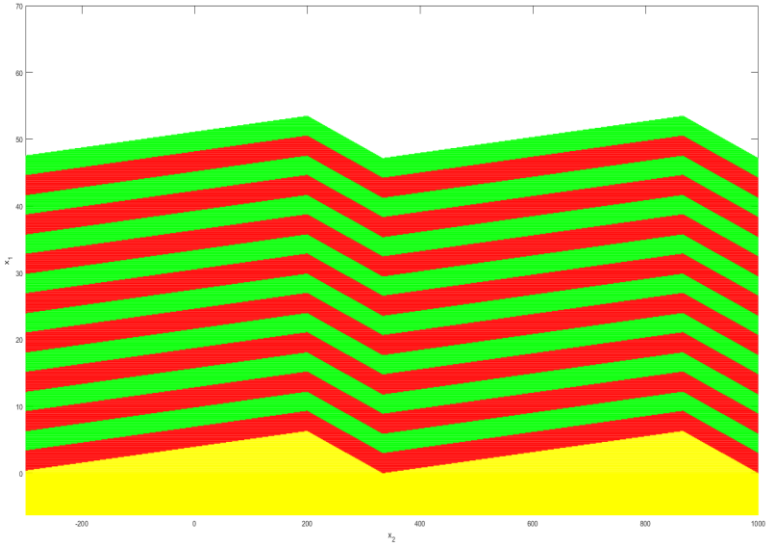
Simulating multilayer blazed gratings

Our code enables the parameters below to be freely varied in order to find the optimised multilayer blazed grating design

Parameter	Description
$D = 1/N$	Grating period
α	Blaze angle
A	Apex angle (A = 180° - α - β)
d	Multilayer period
γ	Width of 1st layer (Cr) in Cr/C multilayer / d
num_periods	Number of multilayer periods
num_slices	Number of slices to define blaze profile
m_max	Maximum diffraction order



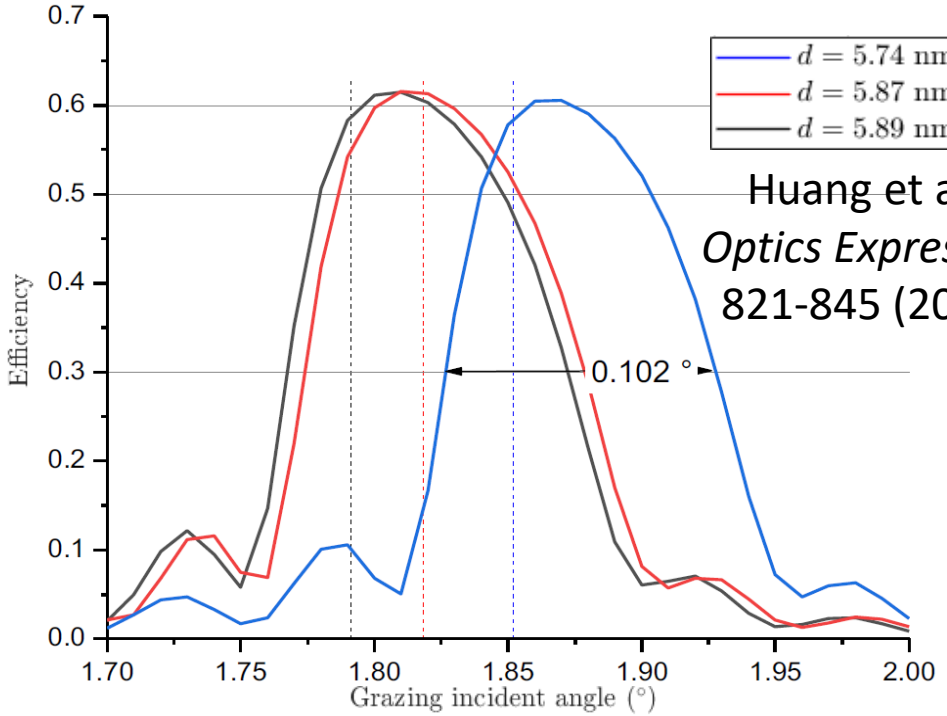
Huang et al., Optics Express **28** 821-845 (2020)



num_slices = 50

Another example: a multilayer blazed grating for I21

Analytical approach



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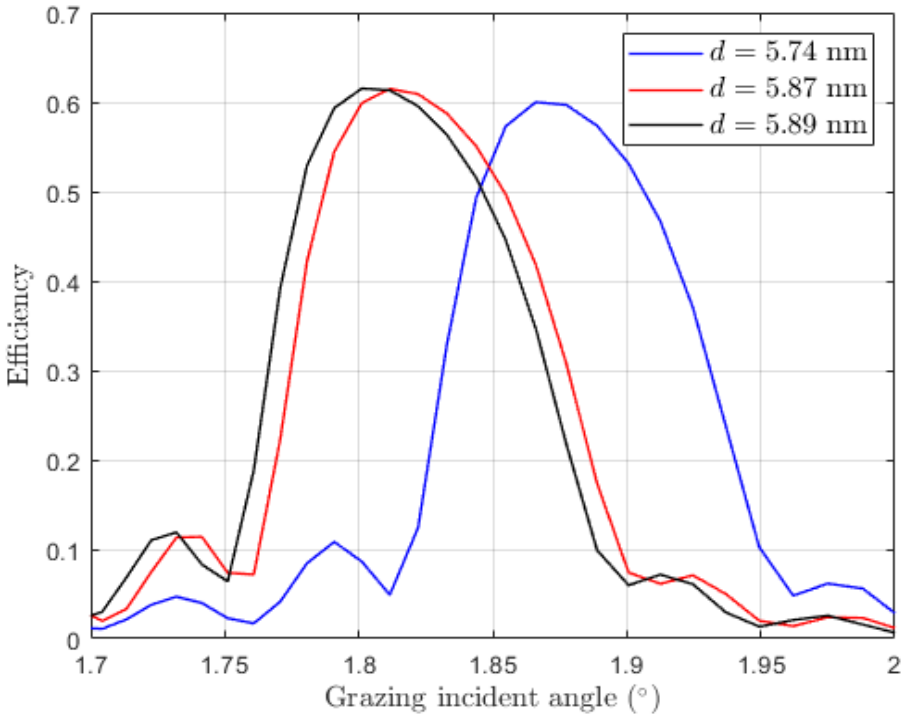
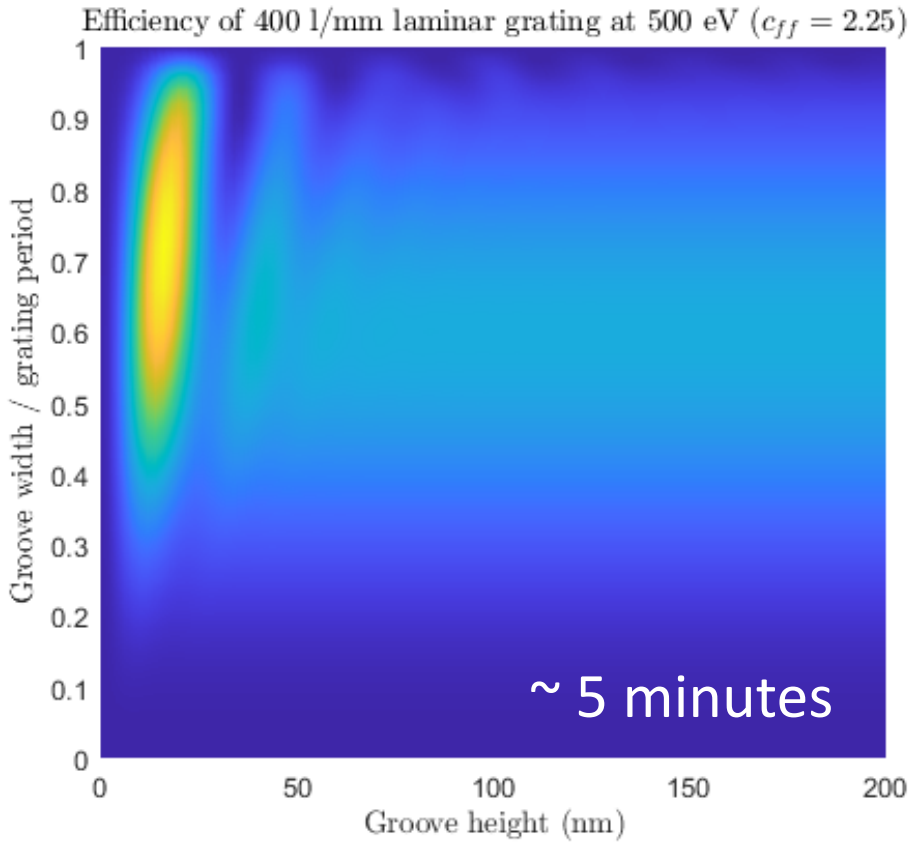
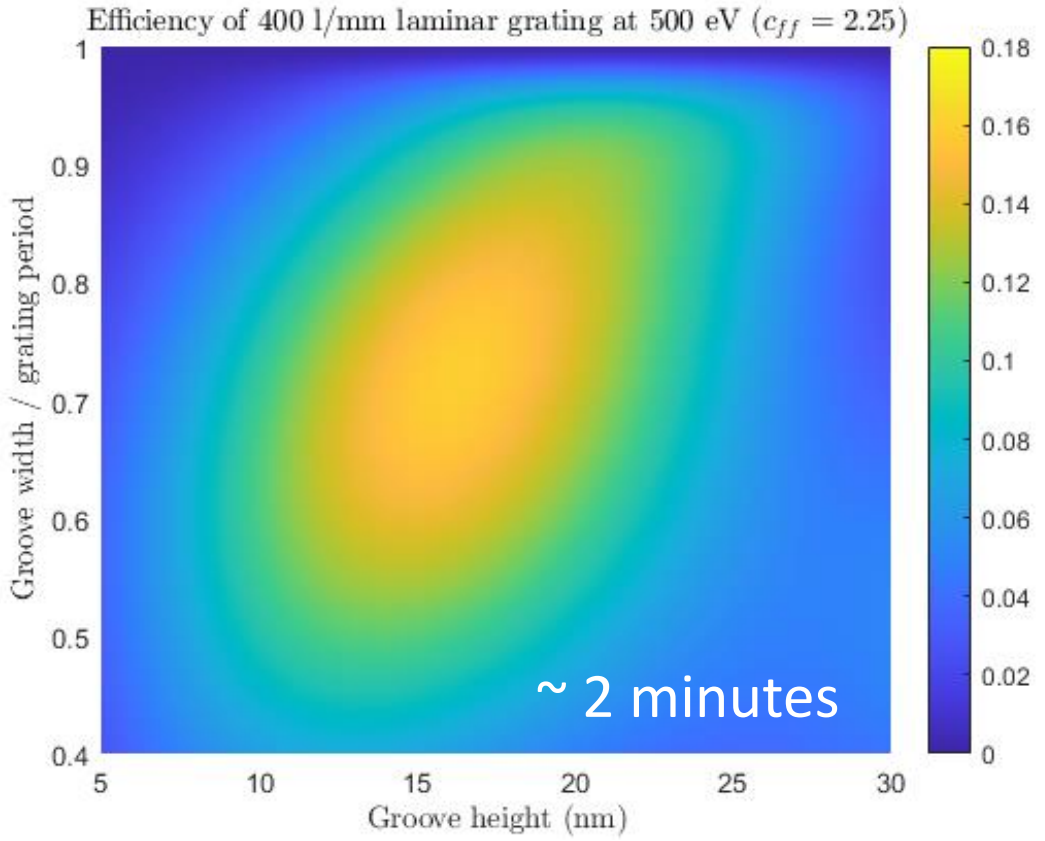
Our results using GD-Calc



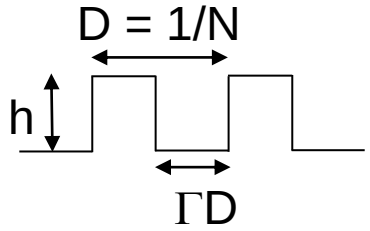
The agreement between the two approaches is excellent!

Using scripting to design new gratings





- Efficient use of time
- Helps ensure that the best combinations of parameters are not overlooked
- Produces pretty pictures in what could otherwise be a relatively boring talk



Summary and future plans

- Our MATLAB software, incorporating GD-Calc, looks very promising as a method to simulate the grating efficiency of both single-layer and multilayer gratings
- The software makes it straightforward to script grating efficiency simulations, speeding up the optimisation of grating designs compared to REFLEC
- The software is available for free (but needs a MATLAB licence to run!)
- MATLAB Compiler could be used to create a standalone program which would not require a MATLAB licence (similar to REFLEC) or to enable the program to be used with other programming languages (such as Python)

If you are interested in using the program,
please let us know how you would like to see it develop!