

#### **Configuration of Grating Structures with Two-Dimensional Periodicity**

#### Abstract



Complex optical grating structures are widely used for several applications such as spectrometers, near-eye display systems, etc. VirtualLab Fusion provides rigorous analysis of arbitrary grating structures in an easy way by applying the Fourier modal method (FMM, also known as RCWA). With the graphical user interface, one can set up the geometry of a stack, so to generate complex grating structures. This use case is focused on the configuration of grating structures which exhibit a two-dimensional periodicity.

### This Use Case Shows ...

- How to configure two-dimensional grating structures in Grating Toolbox by using
  - medium-based definition type
  - interface-based definition type
- How to change advanced options & inspect defined structure before calculation.
- note: In VirtualLab grating structures, which exhibit a two-dimensional periodicity are called 3D gratings. Consequently, lamellar gratings (1Dperiodicity) are called 2D gratings.

## **Grating Toolbox Initialization**

- Initialization
  - Start →
     Grating →
     General Grating Light Path Diagram
     (3D Gratings)
- note: For usage of special type of grating, e.g. pillar grating, the specific light path diagram can be chosen directly.



## **Grating Structure Settings**

- First, the thickness and the material of the substrate (Base Block) have to be defined.
- In VirtualLab grating structures are defined in a so called stack.
- Stacks can be attached to either one or both sides of the substrate.



• For example, a stack on the first interface is chosen.



Medium-based Definition Type (Example: Pillar Grating)

#### **Stack Editor**

- In the Stack Editor, interfaces and media can be added or inserted from catalog.
- In order to define a grating by a special medium, two plane interfaces have to be added, which act as boundaries.

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Z-Extension

Extension

Tools 🍟 🗸 Show Preview

Definition Type Templates — Aphenical Interface — Combined Interface — Conical Interface — Cydnoical Interface — Polynomial Interface — Programmable Interface — Rectangular Grating Interface — Sampled Interface — Sampled Interface

Transition Point List Interface
 Triangular Grating Interface
 Zemike Standard Interface

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#### **Stack Editor**

- The medium between the two plane interfaces can be either homogenous or modulated.
- By using a latter one complex grating structures, like pillar gratings, can be described very efficiently.

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Definition Type Templates
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GRIN Medium
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Volume Grating Medium

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			>
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		Stack Period is Independent from Interface/Media Period V	
		Stack Period 10 µm	
cel Help		Image: Tools marging with the second	۶lp

## **Pillar Grating Medium**

- In the catalog category "LightTrans Defined" the Chromium Pillars can be found in the pillar media category.
- This type of medium enables e.g. the simulation of pillar structure as well as pin holes on top of a substrate.
- In this example, rectangular pillars which consist of chromium are located on a fused silica substrate.
- In the view of the stack editor, different materials are indicated by other colors based on their index of refraction (dark means higher).
- note: The stack editor will always provide a cross-sectional view of the x-z plane.

![](_page_8_Figure_6.jpeg)

#### **Pillar Grating Medium**

- Please note: the order of the interfaces is always counted from the surface of the substrate.
- The selected interface is highlighted in red.
- Further, the medium in front of the grating (means behind last interface) can not be defined here. It is automatically taken from the material in front of the grating component.
- This material can be changed in the Optical Setup Editor.

![](_page_9_Picture_5.jpeg)

![](_page_9_Figure_6.jpeg)

#### **Pillar Grating Medium**

- The Stack Period allows to control the period of the whole configuration.
- In case of a grating exhibiting a twodimensional periodicity the period has to be defined in x- and y-direction.
- This period is also taken for the periodic boundary conditions of the FMM algorithm.
- In case of simple grating structures, it is recommended to choose the option Dependent from the Period of Medium and select the proper index of the periodic medium.

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									× Base Block
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P	eriod Stack F Stack F	<sup>p</sup> eriod is <sup>p</sup> eriod	Dependent f	rom the Period of I	Medium	n ∽ 400 nm	with Index	1	\$
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### **Pillar Grating Medium Parameters**

# The pillar grating is defined by the following parameters:

- base material (material of grooves)
- pillar material (material of ridges)
- shape of pillars (either rectangular or elliptic)
- pillar distance in x-direction (horizontal)
- pillar distance in y-direction (vertical)
- row shift (allows a displacement of rows)
- grating period in x- and y-direction

![](_page_11_Figure_9.jpeg)

dit Pillar Medium (z-Independent) X						
Basic Parameters Scaling Periodization						
Base Material Name Air						
Catalog Material V						
State of Matter Gas or Vacuum ~						
Pillar Material						
Name Chromium-Cr_(1994)						
Catalog Material 🗸 🖉						
State of Matter Solid ~						
Pillar Size and Shape						
Shape 🔿 Rectangular 💿 Elliptic						
Diameter 200 nm x 200 nm						
Horizontal Pillar Distance 400 nm						
Horizontal Pillar Distance 400 nm Vertical Pillar Distance 200 nm						
Horizontal Pillar Distance     400 nm       Vertical Pillar Distance     200 nm       Row Shift     200 nm						
Horizontal Pillar Distance     400 nm       Vertical Pillar Distance     200 nm       Row Shift     200 nm       Period     400 nm						

#### **Pillar Grating Medium Parameters**

- The period of the pillar grating is calculated based on pillar size and distance automatically.
- Thus, it cannot be set individually and the boxes are shown grayed out.

Edit Pillar Medium (z-Independent) X
Basic Parameters Scaling Periodization
Base Material
Name Air Q
Catalog Material 🗸 🧪
State of Matter Gas or Vacuum ~
Pillar Material
Name Chromium-Cr_(1994)
Catalog Material 🗸 🖉
State of Matter Solid ~
Pillar Size and Shape
Shape O Rectangular I Elliptic
Diameter 200 nm x 200 nm
Horizontal Pillar Distance 400 nm
Vertical Pillar Distance 200 nm
Row Shift 200 nm
Period         400 nm         x         400 nm
OK Cancel Help

- In the propagation menu several advanced options are available.
- The propagation method tab allows to edit the accuracy settings of the FMM algorithm.
- Either the numbers of considered total orders or evanescent orders in each direction can be set.
- This might be useful, especially if metallic gratings are considered.
- In contrast, in case of dielectric gratings, the default setting will be sufficient.

![](_page_13_Picture_6.jpeg)

- The Advanced Settings tab provides information about the decomposition of the structure.
- The Layer Decomposition and Transition Point Decomposition settings can be used to adjust the discretization of the structure. The default settings are appropriate for nearly all grating structures.
- Further, information about the number of layers and transition points are provided.
- The Decomposition Preview button provides a depiction of the structure data which are used for the FMM calculation. The refractive index is illustrated by a color scale.

![](_page_14_Picture_5.jpeg)

- The decomposition preview of the defined pillar grating (top view).
- VirtualLab suggests a discretization in 2 layers (1 layer is representing the substrate).

![](_page_15_Figure_3.jpeg)

![](_page_15_Picture_4.jpeg)

Interface-based Definition Type (Example: Truncated Cone Grating)

#### **Stack Editor**

- In the Stack Editor interfaces can be added or inserted from catalog.
- In the category "2D Grating Interface" there are two different interfaces for definition of 3D grating structures.

Definition Type Light Trans Defined - 2D Grating Interfaces

🗑 / X

Truncated Pyramid Grating Interfac - Anamorphic Interfaces - Aspherical Interfaces - Axicon Interfaces - Lens Array Interfaces Miscellaneous 2D Modulated Interfaces - Rotational Symmetric Programmed Interfac Toroidal Interfaces - X-Modulated Interface

× jor

**Z**-Extension Extension

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4 mm Minimum

OK

![](_page_17_Figure_3.jpeg)

- In this example, the "Truncated Cone Grating Interface" is used.
- This type of interface enables e.g. the simulation of anti-reflective structures with a circular shape.
- In this example, cones which are made of fused silica located on a substrate of the same material.
- In the view of the stack editor, different materials are indicated by other colors based on their index of refraction (dark means higher).
- note: The Stack Editor will always provide a cross-sectional view of the x-z plane.

![](_page_18_Figure_6.jpeg)

- Please note: the order of the interfaces is always counted from the surface of the substrate.
- The selected interface is highlighted in red.
- Further, the medium in front of the grating (means behind last interface) can not be defined here. It is automatically taken from the material in front of the grating component.
- This material can be changed in the Optical Setup Editor.

![](_page_19_Picture_5.jpeg)

![](_page_19_Figure_6.jpeg)

- Further, the material of the cones is automatically taken from the material subsequent to the interface.
- In this example, this means, that the material of the substrate (base block) is used.
- If the grating structure is made of a different material, an additional plane interface has to be added in order to separate the grating structure from base block.
- Afterwards, the material between the truncated cone and the plane interface can be chosen as desired.

![](_page_20_Figure_5.jpeg)

- The Stack Period allows to control the period of the whole configuration.
- In case of a grating exhibiting a twodimensional periodicity the period has to be defined in x- and y-direction.
- This period is also taken for the periodic boundary conditions of the FMM algorithm.
- In case of simple grating structures, it is recommended to choose the option Dependent from the Period of Interface and select the proper index of the periodic interface.

![](_page_21_Figure_5.jpeg)

## **Truncated Cone Grating Parameters**

The pillar grating is a programable interface and defined by the following parameters:

- height of cones
- height factor (e.g. allows to invert the structure
- diameter at the top
- diameter at the bottom (base)
- grating period in x- and y-direction
- the materials are automatically set

![](_page_22_Picture_8.jpeg)

Edit Progra	mmable Interface					$\times$
Structure	Height Discontinuities	Scaling of Elemen	tary Interface	Periodization		
Interface Algorith	Specification ms					
Snippe	et for Height Profile		/ E	dit	Validity: 🕑	
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TopDia	ameter					2 µm
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Shape	e 💿 Rec	tangular	O Elliptic			
Size		5 µm x		5 µm		
Effect o	n Field Outside of Defin	ition Area				
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⊖ Fi	eld is Absorbed					
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z-Po	osition	-4 µm		0	z-Position	
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#### **Truncated Cone Grating Parameters**

- As this is a general programmable interface, the grating period has to be set in the periodization tab.
- This means also, that the definition of the grating and its parameters can easily adapted by adjusting the code, which defines the structure.

![](_page_23_Picture_3.jpeg)

	Discontinuities	Scaling of Eleme	ntary Interface	Periodization	
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Position of S	Surrounding Inte	face Plane			
Specificatio	on Mode	8			Def. Area
	Boundary Minir	num 🗸			}₩
z-Position		-4 µm			5
				0 z-Positi	on
dit Inner Definit	on Area				

- Again, in the propagation menu several advanced options are available.
- The propagation method tab allows to edit the accuracy settings of the FMM algorithm.
- Either the numbers of considered total orders or evanescent orders in each direction can be set.
- This might be useful, especially if metallic gratings are considered.
- In contrast, in case of dielectric gratings, the default setting will be sufficient.

![](_page_24_Picture_6.jpeg)

- The Advanced Settings tab provides information about the decomposition of the structure.
- The Layer Decomposition and Transition Point Decomposition settings can be used to adjust the discretization of the structure. The default settings are appropriate for nearly all grating structures.
- Further, information about the number of layers and transition points are provided.
- The Decomposition Preview button provides a depiction of the structure data which are used for the FMM calculation. The refractive index is illustrated by a color scale.

![](_page_25_Picture_5.jpeg)

- The decomposition preview of the defined pillar grating (top view).
- VirtualLab suggests a discretization in 21 layers (1 layer is representing the substrate).

![](_page_26_Figure_3.jpeg)

![](_page_26_Picture_4.jpeg)

By browsing through the different layers, the decomposed structure can be investigated in detail.

 Permosition Preview
 Note: Coordinates are shifted by half a period.
 Note: Coordinates are shifted by half a period.<

![](_page_27_Figure_2.jpeg)

4.5

3.5 4

Υ [µm] 2 2.5 3

 If the numbers of layers and transition points are increased (e.g. by a factor of 2), the discretization becomes smoother, at the expense of increased numerical effort.

![](_page_28_Figure_2.jpeg)

![](_page_28_Picture_3.jpeg)

#### **Remark on the Detector Position**

- In VirtualLab the detector is located subsequent to the substrate in air by default.
- This is necessary if the grating is included in a complex optical setup.
- However, the perfect plane and parallel substrate may cause some interference effects, which not occur in reality.
- Thus, for calculation of just grating efficiencies it is appropriate to set the detector inside the substrate material (likewise to most of grating evaluation software).
- This avoids the undesired influence of those interference effects.

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document code	MISC.0050
version	1.1
toolbox(es)	Grating Toolbox
VL version used for simulations	7.4.0.49
category	Feature Use Case
further reading	<ul> <li><u>Configuration of Grating Structures by Using Interfaces</u></li> <li><u>Configuration of Grating Structures by Using Special Media</u></li> </ul>