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**Physical-optics modeling of diffractive and meta-lenses and their design**

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Emphasis of the common theoretical background for different types of microstructured layers
Wavefront Surface Response Function

Unifying approach for dealing with different structure concepts in optical modeling and design
Plane Wave Interaction with Plane Surface

- For a field in a plane we use the notation $\rho = (x, y)$ and $V_{\perp}(\rho) = (E_x(\rho), E_y(\rho))$.

- A plane input field is given by

$$V_{\perp}^{\text{in}}(\rho) = U_{\perp}^{\text{in}} \exp(i\kappa^{\text{in}} \rho)$$

with $\kappa = (k_x, k_y)$.

- The transmitted plane output field is given by

$$V_{\perp}^{\text{out}}(\rho) = (B(\kappa^{\text{in}})U_{\perp}^{\text{in}}) \exp(i\kappa^{\text{out}} \rho)$$

with the Fresnel effect at the surface is expressed by the $2 \times 2$ matrix $B(\kappa^{\text{in}})$.

- From the boundary conditions follows: $\kappa^{\text{out}} \perp \kappa^{\text{in}}$
Plane Wave Interaction with Plane Surface

- From the boundary conditions follows: $\kappa^\text{out} \overset{!}{=} \kappa^\text{in}$

- With $\kappa = k_0 n \hat{s}_\perp = k_0 n (\sin \theta \cos \phi, \sin \theta \cos \phi)$ and $\phi = 0$ the law of refraction follows: $n^\text{in} \sin \theta^\text{in} = n^\text{out} \sin \theta^\text{out}$.

- For plane wave fields the wavefront phase is given by $\psi(\rho) = \kappa \cdot \rho$.

- With $\kappa^\text{out} \overset{!}{=} \kappa^\text{in}$ we conclude $\psi^\text{out}(\rho) = \psi^\text{in}(\rho)$.

- With $\nabla_\perp = \left\{ \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right\}$ we find for plane wave fields:

$$\kappa = \nabla_\perp \psi(\rho)$$

- Then $\kappa^\text{out} \overset{!}{=} \kappa^\text{in}$, that is the law of refraction, can be expressed by $\nabla_\perp \psi^\text{in}(\rho) = \nabla_\perp \psi^\text{out}(\rho)$. 
General Field Interaction with Plane Surface

- Consider a general input field $V_{\perp}^{\text{in}}(\rho) = U_{\perp}^{\text{in}}(\rho) \exp(i\psi_{\text{in}}^{\text{in}}(\rho))$.

- In general the effect of the plane surface on the input field can be expressed by the operator equation $V_{\perp}^{\text{out}}(\rho) = \mathcal{B}V_{\perp}^{\text{in}}(\rho)$.

- Next we assume that we are allowed to apply the plane wave results locally. In physical optics that means the fields are in its homeomorphic field zone (HFZ).

- In the homeomorphic field zone we can express the effect of the plane surface on the input field locally:

$$U_{\perp}^{\text{out}}(\rho) \exp(i\psi_{\text{out}}^{\text{out}}(\rho)) = \mathcal{B}(\rho) \{U_{\perp}^{\text{in}}(\rho) \exp(i\psi_{\text{in}}^{\text{in}}(\rho))\}$$

- The local use of the law of refraction can be expressed by:

$$\nabla_{\perp} \psi_{\text{in}}^{\text{in}}(\rho) = \nabla_{\perp} \psi_{\text{out}}^{\text{out}}(\rho)$$
General Field Interaction with Plane Surface

- In the homeomorphic field zone we can express the effect of the plane surface on the input field locally:

\[ U_{\perp}^{\text{out}}(\rho) \exp(i\psi_{\text{out}}(\rho)) = B(\rho) \{ U_{\perp}^{\text{in}}(\rho) \exp(i\psi_{\text{in}}(\rho)) \} \]

- The local use of the law of refraction is expressed by:

\[ \nabla_{\perp} \psi_{\text{in}}(\rho) = \nabla_{\perp} \psi_{\text{out}}(\rho) \]

- In conclusion the effect on the phase is described by the local Fresnel effects:

\[ U_{\perp}^{\text{out}}(\rho) \exp(i\psi_{\text{in}}(\rho)) = \{ B(\rho; \psi_{\text{in}}) U_{\perp}^{\text{in}}(\rho) \} \exp(i\psi_{\text{in}}(\rho)) \]
General Field Interaction with Plane Surface

- Intermediate result: Plane surfaces do not change the wavefront phase of the incident field.
General Field Interaction with Curved Surface

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- For curved surfaces the modeling can be still applied locally. Then the wavefront phase can be shaped by the shape of the surface:

\[ \psi^{\text{out}}(\rho) \neq \psi^{\text{in}}(\rho) \]
General Field Interaction with Curved Surface

- Intermediate result: Plane surfaces do not change the wavefront phase of the incident field.

- For curved surfaces the modeling can be still applied locally. Then the wavefront phase can be shaped by the shape of the surface:

\[ \psi^{\text{out}}(\rho) \neq \psi^{\text{in}}(\rho) \]

- In what follows a change of the wavefront phase should be enforced by assuming a Wavefront Response Function \( \Delta \psi(\rho) \) instead of (in addition to) a curved surface.
Wavefront Surface Response (WSR)

- For plane surfaces we found $\nabla_{\perp} \psi^\text{in}(\rho) = \nabla_{\perp} \psi^\text{out}(\rho)$ and in conclusion

$$U_{\perp}^\text{out}(\rho) \exp(i\psi^\text{in}(\rho)) = \{B(\rho; \psi^\text{in})U_{\perp}^\text{in}(\rho)\} \exp(i\psi^\text{in}(\rho)).$$
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U^{\text{out}}_\perp(\rho) \exp(i\psi^{\text{in}}(\rho)) = \{ B(\rho; \psi^{\text{in}}) U^{\text{in}}_\perp(\rho) \} \exp(i\psi^{\text{in}}(\rho)) .
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- By introducing the wavefront surface response we assume an effect at the surface of the form
  $$U^{\text{out}}_\perp(\rho) \exp(i\psi^{\text{out}}(\rho)) = \{ \mathbf{B}(\rho; \psi^{\text{in}}) U^{\text{in}}_\perp(\rho) \} \exp(i\psi^{\text{out}}(\rho))$$

  with
  $$\psi^{\text{out}}(\rho) = \psi^{\text{in}}(\rho) + \Delta \psi(\rho)$$

  and thus
  $$\nabla_\perp \psi^{\text{out}}(\rho) = \nabla_\perp \psi^{\text{in}}(\rho) + \nabla_\perp (\Delta \psi(\rho)).$$
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with

$$\psi^{\text{out}}(\rho) = \psi^{\text{in}}(\rho) + \Delta \psi(\rho)$$

and thus

$$\nabla_{\perp} \psi^{\text{out}}(\rho) = \nabla_{\perp} \psi^{\text{in}}(\rho) + \nabla_{\perp} (\Delta \psi(\rho)) .$$
Wavefront Surface Response (WSR)

- Because of the local plane wave assumption (homeomorphic zone)
  \[ \nabla_{\perp} \psi^{\text{out}}(\rho) = \nabla_{\perp} \psi^{\text{in}}(\rho) + \nabla_{\perp} (\Delta \psi(\rho)) \]

  leads to
  \[ \kappa^{\text{out}}(\rho) = \kappa^{\text{in}}(\rho) + K(\rho) \]

  with \( K(\rho) \defeq \nabla_{\perp} (\Delta \psi(\rho)) \).

- That gives a direct access to ray tracing with \( \kappa(\rho) = k_0 n \hat{s}_{\perp}(\rho) \) via
  \[ n^{\text{out}} \hat{s}_{\perp}(\rho) = n^{\text{in}} \hat{s}_{\perp}(\rho) + K(\rho)/k_0. \]
How to Realize a Desired Wavefront Surface Response (WSR)?

- From a physical-optics point of view the question arises, if there exists any manipulation of the structure of the surface, which provides an effect of the form:

$$U_{\text{out}}(\rho) \exp(i\psi_{\text{in}}(\rho) + \Delta\psi(\rho)) = \left\{B(\rho; \psi_{\text{in}})U_{\text{in}}(\rho)\right\} \exp(i\psi_{\text{in}}(\rho))$$

- A detailed answer can only be given for a specific surface structure.

- By introducing microstructured layers onto the surface a wavefront surface response can be implemented:
  - Graded-index layer
  - Volume hologram layer
  - Diffractive layer
  - Metamaterial layer
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Metasurfaces

Realization of wavefront surface responses by nanostructured layers
Physical Effects for Realizing Metasurfaces

• Propagation phase delay
  - Centrosymmetric (polarization insensitive)
  - Rotationally asymmetric (form birefringence)


• Resonance phase delay

Y. F. Yu et al., Laser Photonics Rev. 9, 412-418 (2015).
Physical Optics Modeling: Metasurface Layer

• In general a real surface layer structure does not just realize the desired wavefront response but additional effects and fields:

\[
V_{\text{out}}(\rho) = \left\{ B(\rho; \psi_{\text{in}})U_{\perp}^{\text{in}}(\rho) \right\} \exp(i\psi_{\text{in}}(\rho) + \Delta\psi(\rho)) + V_{\perp}^{\text{res}}(\rho)
\]

• For nanofin-based metalayers the typical result can be written as:

\[
V_{\perp}^{\text{out}}(\rho) = \left\{ B^+(\rho; \psi_{\text{in}})U_{\perp}^{\text{in}}(\rho) \right\} \exp(i\psi_{\text{in}}(\rho) + \Delta\psi(\rho)) + \left\{ B^- (\rho; \psi_{\text{in}})U_{\perp}^{\text{in}}(\rho) \right\} \exp(i\psi_{\text{in}}(\rho) - \Delta\psi(\rho))
\]

Physical Optics Modeling: Metasurface Layer

- In general a real surface layer structure does not just realize the desired wavefront response but additional effects and fields:

\[ V_{\text{out}}^{\perp}(\rho) = \{ B^{\perp}(\rho; \psi^{\text{in}}) U^{\text{in}}_{\perp}(\rho) \} \exp(i\psi^{\text{in}}(\rho) + \Delta\psi(\rho)) + V_{\text{res}}^{\perp}(\rho) \]

- For nanofin-based metalayer as:

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+ \{ B^{-}(\rho; \psi^{\text{in}}) U^{\text{in}}_{\perp}(\rho) \} \exp(i\psi^{\text{in}}(\rho) - \Delta\psi(\rho))
\]

Calculation by Fourier modal method (FMM), a.k.a. RCWA

Metasurface Building Block

- Building blocks over the whole surface are same, but with different rotation angle $\theta(\rho)$. That can be expressed as

$$V_{\text{out}}^{\perp}(\rho) = \begin{pmatrix} \cos \theta(\rho) & -\sin \theta(\rho) \\ \sin \theta(\rho) & \cos \theta(\rho) \end{pmatrix} \begin{pmatrix} b_{xx} & b_{xy} \\ b_{yx} & b_{yy} \end{pmatrix} \begin{pmatrix} \cos \theta(\rho) & \sin \theta(\rho) \\ -\sin \theta(\rho) & \cos \theta(\rho) \end{pmatrix} V_{\text{in}}^{\perp}(\rho)$$

... in the “eigen” coordinate system of each nanofin
Metasurface Building Block

Calculation by Fourier modal method (FMM), a.k.a. RCWA

\[
\begin{align*}
V_{\perp}^{\text{out}}(\rho) &= \begin{pmatrix} \cos \theta(\rho) & -\sin \theta(\rho) \\ \sin \theta(\rho) & \cos \theta(\rho) \end{pmatrix} \begin{pmatrix} b_{xx} & b_{xy} \\ b_{yx} & b_{yy} \end{pmatrix} \begin{pmatrix} \cos \theta(\rho) \\ -\sin \theta(\rho) \end{pmatrix} V_{\perp}^{\text{in}}(\rho)
\end{align*}
\]

... in the “eigen” coordinate system of each nanofin
Physical Optics Modeling: Metasurface Layer

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\[ V_{\perp}^{\text{out}}(\rho) = \{ B(\rho; \psi^{\text{in}}) U_{\perp}^{\text{in}}(\rho) \} \exp(i\psi^{\text{in}}(\rho) + \Delta \psi(\rho)) + V_{\perp}^{\text{res}}(\rho) \]

- For nanofin-based metalayers the typical result can be written as:

\[ V_{\perp}^{\text{out}}(\rho) = \{ B^+(\rho; \psi^{\text{in}}) U_{\perp}^{\text{in}}(\rho) \} \exp(i\psi^{\text{in}}(\rho) + \Delta \psi(\rho)) \]
\[ + \{ B^-(\rho; \psi^{\text{in}}) U_{\perp}^{\text{in}}(\rho) \} \exp(i\psi^{\text{in}}(\rho) - \Delta \psi(\rho)) \]

- In depth investigation reveals, that \(+\Delta \psi\) occurs for R-circularly polarized input fields and the conjugate phase for L-circularly polarized input.

Metasurface layer

Linear Wavefront Response Function
Plane Wave through Plate: Ray and Field Tracing

Law of refraction
Plane Wave through Plate: Introducing Metasurface

\[ \Delta \psi(\rho) = \kappa_{\text{meta}} \cdot \rho \]
Propagation Plate with Metasurface: Ray and Field Tracing

\[ \Delta \psi(\rho) = \kappa_{\text{meta}} \cdot \rho \]
Propagation Plate with Metasurface: Ray and Field Tracing

\[ \Delta \psi(\rho) = \kappa_{\text{meta}} \cdot \rho \]
Plane Wave through Plate: Ray and Field Tracing

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Plate with Metasurface: Ray and Field Tracing

\[ \Delta \psi(\rho) = \kappa_{\text{meta}} \cdot \rho \]
Plate with Metasurface: Ray and Field Tracing

Left circularly polarized

$$\Delta \psi(\rho) = \kappa_{\text{meta}} \cdot \rho$$
Plate with Metasurface: Ray and Field Tracing

\[ \Delta \psi (\rho) = \kappa_{\text{meta}} \cdot \rho \]
Polarization Dependent Function of Nanofin Metalayer

\[ V_{\perp}^{\text{out}}(\rho) = \{ B^+(\rho; \psi^{\text{in}}) U^{\text{in}}_{\perp}(\rho) \} \exp(i\psi^{\text{in}}(\rho) + \Delta\psi(\rho)) \]

\[ + \{ B^-(\rho; \psi^{\text{in}}) U^{\text{in}}_{\perp}(\rho) \} \exp(i\psi^{\text{in}}(\rho) - \Delta\psi(\rho)) \]

Linear Polarized (Ex) Right Circularly Polarized Left Circularly Polarized
Polarization Dependent Function of Nanofin Metalayer

Elliptical Polarization:

\[
\begin{pmatrix}
J_x \\
J_y
\end{pmatrix} = \begin{pmatrix}
0.59957 \\
0.13531 + i0.7888
\end{pmatrix}
\]
High-NA Metalens Simulation

input plane wave
- normal incidence
- wavelength @ 532 nm
- beam diameter 2 mm
- polarization state
  a) R-circular
  b) Linear
  c) L-circular

\[ \Delta \psi(\rho) = k_0 n \left( f - \sqrt{||\rho||^2 + f^2} \right) \]

Desired to function as a focusing lens

How to calculate the point spread function (PSF) at the focal plane of a metalens, with polarization effects considered?

High-NA Metalens Simulation

\[ V_{\perp}^{\text{out}}(\rho) = \{ B^+(\rho; \psi^{\text{in}}) U_{\perp}^{\text{in}}(\rho) \} \exp(i\psi^{\text{in}}(\rho) + \Delta\psi(\rho)) + \{ B^- (\rho; \psi^{\text{in}}) U_{\perp}^{\text{in}}(\rho) \} \exp(i\psi^{\text{in}}(\rho) - \Delta\psi(\rho)) \]

- Only desired mode
- Both desired and conjugate modes
- Only conjugate mode
High-NA Metalens Simulation

$$V_{\perp}^{\text{out}}(\rho) = \{B^+(\rho; \psi^\text{in})U_{\perp}^{\text{in}}(\rho)\} \exp(i\psi^\text{in}(\rho) + \Delta\psi(\rho))$$

$$+ \{B^-(\rho; \psi^\text{in})U_{\perp}^{\text{in}}(\rho)\} \exp(i\psi^\text{in}(\rho) - \Delta\psi(\rho))$$

FWHM = 355µm

2µm

R-circular polarization input
linear polarization input
L-circular polarization input
Diffractive layer

... with application to lenses
Physical Optics Modeling: Diffractive Layer

- In general a wavefront surface response $\Delta \psi(\rho)$ leads to the equation $\nabla_\perp \psi^\text{out}(\rho) = \nabla_\perp \psi^\text{in}(\rho) + \nabla_\perp (\Delta \psi(\rho))$ and because of the local plane wave assumption (homeomorphic zone) into

$$\kappa^\text{out}(\rho) = \kappa^\text{in}(\rho) + K(\rho)$$

with $K(\rho) \overset{\text{def}}{=} \nabla_\perp (\Delta \psi(\rho))$.

- This equation is directly related to a locally formulated grating equation

$$\kappa^\text{out}(\rho) = \kappa^\text{in}(\rho) + m \left( \frac{2\pi}{d_x(\rho)}, \frac{2\pi}{d_y(\rho)} \right)$$

with the local grating period $d(\rho) = (d_x(\rho), d_y(\rho))$.

- That leads to the basic principle of a diffractive layer via:

$$d(\rho) = 2\pi \left( \left( \frac{\partial \psi(\rho)}{\partial x} \right)^{-1}, \left( \frac{\partial \psi(\rho)}{\partial y} \right)^{-1} \right)$$
Physical Optics Modeling: Diffractive Layer

• This design and modeling understanding results in the decomposition of the output field into a series of local grating orders:

\[
V_{\perp}^{out}(\rho) = \left\{ B^{(1)}(\rho; \psi^{in})U^{in}_{\perp}(\rho) \right\} \exp(i\psi^{in}(\rho) + \Delta\psi(\rho))
\]

\[
+ \sum_{m=-\infty, m\neq 1}^{\infty} \left\{ B^{(m)}(\rho; \psi^{in})U^{in}_{\perp}(\rho) \right\} \exp(i\psi^{in}(\rho) + m\Delta\psi(\rho))
\]

• The $2 \times 2$ matrix $B^{(m)}(\rho; \psi^{in})$ expresses the Rayleigh-matrix of grating theory and is rigorously calculated per direction and period by the Fourier Modal Method (FMM). Design should minimize Rayleigh coefficients for all undesired orders.

• Complications: Period drastically varies over surface, which results in a laterally varying number of propagating subfields. Full treatment available in **VirtualLab Lens Solutions**.
Wavefront Surface Response of Focusing Lens

- In order to transform a plane incident field into a spherical convergent one the wavefront surface response should be:

\[ \Delta \psi(\rho) = k_0 n \left( f - \sqrt{||\rho||^2 + f^2} \right) \]
Structure Design

- Wrap the WSR: \((\Delta \psi(\rho))^{DOE} = \text{mod}_{p2\pi} \left\{ k_0 n \left( f - \sqrt{||\rho||^2 + f^2} \right) \right\} \) with \(p \in \mathbb{N}\).

- For \(p = 1\) local radial period follows with \(d(\rho) = 2\pi / \Delta \psi'(\rho)\).

- Structure design by inverse Thin Element Approximation (TEA): The height profile \(h^{DOE}\) is given by:

\[
h^{DOE}(\rho) = \frac{\lambda}{2\pi \Delta n} \Delta \psi(\rho)^{DOE}
\]
Focusing Diffractive Lens with NA=0.2: Ray and Field Tracing
Focusing Diffractive Lens with NA=0.2: Ray and Field Tracing

Amplitude

Phase

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Focusing Diffractive Lens with NA=0.2: Ray and Field Tracing

Amplitude

Effects due to Rayleigh matrix:

\[ B(\rho; \psi^{\text{in}}) U_{\perp}^{\text{in}}(\rho) \]

Phase
Focusing Diffractive Lens with NA=0.2: Ray and Field Tracing

- Amplitudes in Focus (Same scaling!)
Focusing Diffractive Lens with NA=0.57: Ray and Field Tracing
Focusing Diffractive Lens with NA=0.57: Ray and Field Tracing

Amplitude

Phase
Focusing Diffractive Lens with NA=0.57: Ray and Field Tracing

Effects due to Rayleigh matrix:

$$B(\rho; \psi^\text{in}) U^\text{in}(\rho)$$
Focusing Diffractive Lens with NA=0.57: Ray and Field Tracing

- Amplitudes in Focus (Same scaling!)
Focusing Diffractive Lens with NA=0.57: Ray and Field Tracing

- Vectorial grating effects reduce spot quality for high NA

- Amplitudes in Focus (Same scaling!)
Lens with NA=0.1 and 8 Height Values: Ray and Field Tracing
Inclusion of Higher Orders

\[ \mathbf{V}_{\perp}^{\text{out}}(\rho) = \left\{ \mathbf{B}^{(1)}(\rho; \psi_{\text{in}}) \mathbf{U}_{\perp}^{\text{in}}(\rho) \right\} \exp(i\psi_{\text{in}}(\rho) + \Delta \psi(\rho)) + \sum_{m=-\infty, m \neq 1}^{\infty} \left\{ \mathbf{B}^{(m)}(\rho; \psi_{\text{in}}) \mathbf{U}_{\perp}^{\text{in}}(\rho) \right\} \exp(i\psi_{\text{in}}(\rho) + m\Delta \psi(\rho)) \]
Inclusion of Higher Orders
Lens with NA=0.1 and 8 Height Values: Ray and Field Tracing

Higher orders have low energy and are defocused in focal region of 1st order: No detrimental effect
Combination of OpticStudio® and VirtualLab Fusion

Complementary workflows
Standard Workflow

- Design of system with optional inclusion of ideal Wavefront Surface Response (WSR) function.
- Decision about most suitable flat optics layer to realize WSR.
- Design of layer structure.
- Analysis of the performance and detrimental additional subfields.
- Tolerancing.
- Export of fabrication data.

Standard Workflow

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Combination with OpticStudio® via Binary Surfaces, which represent a special form of a WSR.

Color Aberration Correction by DOE

- detectors
  - point spread function
  - modulation transfer function (MTF)

- lens solution
  - wavefront response function
  - diffractive lens
  - meta lens

- Optimization of Binary Surface = Wavefront Surface Response in OpticStudio®

- plane wave
  - wavelength (486, 587, 656) nm
  - field of view along y-axis (0; 20)°
  - linearly polarized along x-axis
  - aperture 5 mm × 5 mm

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Standard Workflow

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Import into VirtualLab Fusion and perform design.
Standard Workflow

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• Decision about most suitable flat optics layer to realize WSR.
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Analysis in VirtualLab Fusion.
Inclusion of Higher Orders: On-Axis

Electric Energy Density $[1E6 \, (V/m)^2]$

Electric Energy Density $[1E3 \, (V/m)^2]$

Electric Energy Density $[(V/m)^2]$

Simulation time per order ~seconds

+1st diffraction order

0th diffraction order

-1st diffraction order
Results: MTF for Various Diffractive Lens Structures

MTF w/o DOE

MTF w/ DOE: Continuous, 8, and 4 levels

MTF w/ DOE: Binary
VirtualLab Meta- and Diffractive Surface Solutions

• We prepare a new VirtualLab product for design and modeling meta- and diffractive surfaces to be released in 2019.
• It will be based on the theory presented in this talk. The examples shown in this talk will be included as special Use Cases together with suitable workflows.