Micro-Optics: Theory
Hans Peter Herzig

- Complex amplitude transmittance (paraxial theory)
- Propagation
- Calculation of the phase function $\Phi(x,y)$
- Implementation
- Diffraction efficiency
- Refraction - diffraction properties
- Design example
- Limits of paraxial theory - rigorous theory
- System design

Plane wave

Plane wave: $U_1(z) = ae^{-ikz}$ with $k = 2\pi/\lambda$.

wavefront: $(kz) = \text{constant}$
Complex amplitude transmittance
(thin element approximation)

\[ t(x) = e^{-i\Phi(x)} \]

with \( \Phi(x) = d(x)(n - 1)\left(\frac{2\pi}{\lambda}\right) \)

\[ U_{out}(x) = t(x)U_{in}(x) \mid_{z=0} \]

Thin element approximation - rigorous diffraction theory

The interaction of light with structures having geometrical features in the order of the wavelength cannot be described with classical scalar (thin-) diffraction models, but ask for solutions based on Maxwell's equations.
Propagation of light through thin optical elements

\[ U_{\text{out}}(x, y) = t(x, y)U_{\text{in}}(x, y) \mid_{z=0} \]

\[ \Phi_{\text{out}}(x, y) = \Phi_{\text{in}}(x, y) + \Phi(x, y) \]

\[ \frac{\partial}{\partial x} \Rightarrow \text{x-direction} \]

\[ \frac{\partial}{\partial y} \Rightarrow \text{y-direction} \]
Calculation of the phase function

A thin phase element that is illuminated by an incident wave \( \Phi_{in}(x,y) \) generates an output wave \( \Phi_{out}(x,y) \). The wavefront conversion is described by

\[
\Phi_{out}(x,y) = \Phi_{in}(x,y) + \Phi(x,y)
\]

\[
\Phi(x,y) = \Phi_{out}(x,y) - \Phi_{in}(x,y)
\]

Phase of spherical or plane waves

Diffractive lens which connects an object point \((x_1,y_1,z_1)\) with an image point \((x_2,y_2,z_2)\).

\[
\Phi_i(x,y) = \frac{2\pi}{\lambda} \sqrt{(x-x_1)^2 + (y-y_1)^2 + z_1^2}
\]

Plane wave inclined in the xz-plane:

\[
\phi(x) = \frac{2\pi}{\lambda} \sin(\theta)x
\]
General case

In general, the optical task is more complex, e.g., if an extended object has to be imaged. In that case, the DOE phase function $\Phi(x,y)$ is typically described by a polynomial:

$$
\Phi(x,y) = \frac{2\pi}{\lambda} \sum_{m,n} a_{mn} x^m y^n
$$

The DOE is then optimized by optimizing the polynomial coefficients $a_{mn}$.

Propagation: Angular spectrum

$U(x,y,z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U(x,y) \exp\left[-i2\pi (px x + py y)\right] \exp\left[ikz z\right] dp_x dp_y$

avec $k_z = 2\pi \sqrt{\frac{1}{\lambda^2} - p_x^2 - p_y^2}$
Implementation of the phase function as DOE

In order to realize a diffractive element, the phase function $\Phi$ is wrapped to an interval between 0 and an integer multiple of $2\pi$.

Phase profile: $\Psi(x,y) = \lfloor \Phi(x,y) \rfloor \mod 2\pi$

Relief profile: $h(x,y) = \Psi(x,y) \frac{\lambda_0}{2\pi(n-1)}$

- $n$ refractive index of the grating material
- $\lambda_0$ design wavelength.
refractive

diffractive

\[ \Phi(x) \]
\[ \Psi(x) \]
Binary and continuous-relief DOEs

(a)

(b)

(c)

Diffraction efficiency $\eta$

$$\eta = \frac{P_1}{\sum P_m}$$

$$\eta_{overall} = \frac{P_1}{P_{in}}$$

R: reflection
A: absorption
S: scattering
**Diffraction efficiency** (scalar theory, no losses)

Blazed grating: $\phi_0 = 2\pi$

\[
|A_n| = \frac{1}{N} \sin \left( \frac{\pi}{N} \right) \frac{\sin \left( \frac{n(n-1)}{N} \right)}{\sin \left( \frac{n-1}{N} \right)},
\]

\[
|A_1|^2 = \left( \frac{N}{\pi} \sin \left( \frac{\pi}{N} \right) \right)^2.
\]

N: number of phase levels
n: diffraction order

<table>
<thead>
<tr>
<th>N</th>
<th>2</th>
<th>4</th>
<th>8</th>
<th>16</th>
</tr>
</thead>
<tbody>
<tr>
<td>$</td>
<td>A_1</td>
<td>^2$</td>
<td>40.5%</td>
<td>81.1%</td>
</tr>
</tbody>
</table>

---

**Diffr. efficiency: theory - experiment**

A. Schilling
Diffraction efficiency versus wavelength

\[ \eta(\lambda) = \left( \frac{\sin\left(\frac{\pi}{\lambda_0} \left( \frac{\lambda_0}{\lambda} - m \right) \right)}{\pi \left( \frac{\lambda_0}{\lambda} - m \right)} \right)^2 \]

Swanson, 1989

\[ \eta_{poly} = \frac{\lambda_{max}}{\lambda_{max} - \lambda_{min}} \int_{\lambda_{min}}^{\lambda_{max}} \eta(\lambda) d\lambda \]

Buralli and Morris, 1992

Refraction - Diffraction
Discussion of optical properties

refractive

diffractive
**Refraction**

\[ n_1(\lambda) \sin \theta_1 = n_2(\lambda) \sin \theta_2 \]

**Diffraction**

\[ \sin \theta = m \frac{\lambda}{\Lambda} \]
**Diffraction**

\[ \sin \theta = m \frac{\lambda}{\Lambda} \]

Plane wave

**Refractive-diffractive properties of blazed grating (shrinkage error 10%)**

![Graph showing refractive/diffractive properties](image)
Refractive - diffractive optical elements

- The optical function of an ideal diffractive element is encoded as lateral position of zones.

- If the phase profile of the zones shrinks, the lateral position stays at the same place. Therefore, diffractive elements are insensitive to shrinkage errors.

- Refractive elements are encoded as optical path difference.

- If the profile of the element shrinks, then the optical path length changes also.

Dispersion

Refraction

\[ n = \frac{\lambda}{\Delta \theta} \]

\[ \nu_r = \frac{\theta}{\Delta \theta} = \frac{n_d - 1}{n_F - n_C} \]

\[ \lambda_d = 587.6 \text{ nm} \]
\[ \lambda_F = 486.1 \text{ nm} \]
\[ \lambda_C = 656.3 \text{ nm} \]

Diffraction

\[ \nu_r = \frac{\theta}{\Delta \theta} = \frac{\lambda_d}{\lambda_F - \lambda_C} \]
## Dispersion

<table>
<thead>
<tr>
<th>Abbe number:</th>
<th>Refractive</th>
<th>Diffractive</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nu_r = \frac{n(\lambda_1) - 1}{n(\lambda_2) - n(\lambda_3)}$</td>
<td>$\nu_d = \frac{\lambda_1}{\lambda_2 - \lambda_3}$</td>
<td></td>
</tr>
<tr>
<td>$\lambda_1 = 587.6$ nm</td>
<td>$\nu_r = 80$ to 20</td>
<td>$\nu_d = -3.45$</td>
</tr>
<tr>
<td>$\lambda_2 = 486.1$ nm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$\lambda_3 = 656.3$ nm</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Dispersion ratio $D_r = \frac{\nu_{\text{refractive}}}{\nu_{\text{diffractive}}}$
Paraxial properties of lenses

\[ f_r(\lambda) = \frac{1}{n(\lambda) - 1} \frac{1}{c_1 - c_2} \quad f_d(\lambda) = f_0 \frac{\lambda_0}{\lambda} \]

Spherical aberration \( S_i = (NA)^4 f C_i \)

\[ C_a = \frac{n^2}{(n - 1)^2} \quad C_b = \frac{n^3 - 2n^2 + 2}{n(n - 1)^2} \quad C_c = 1 - \left(\frac{\lambda_d}{\lambda}\right)^2 \]

Numerical aperture \( NA = n_0 \sin \theta \)

Resolution \( \frac{\lambda}{2NA} \)
Airy disk radius

<table>
<thead>
<tr>
<th>Refractive</th>
<th>Diffractive</th>
</tr>
</thead>
<tbody>
<tr>
<td>[r(\lambda) = 1.22 \frac{\lambda f}{D}]</td>
<td>[r(\lambda) = 1.22 \frac{\lambda_0 f_0}{D} \approx \text{const}]</td>
</tr>
</tbody>
</table>

Diffractive elements
- Arbitrary shape
- Accurate focal length
- High functionality
- High dispersion (<0)
- Problems:
  - low NA (< 0.2)
  - diffraction efficiency (80% - 95%)
  - stray-light

Refractive elements
- Spherical and cylindrical shape
- High NA (> 0.1)
- Low dispersion (>0)
- High efficiency
- Low stray-light
- Problems:
  - fill factor
  - arbitrary shapes
Optimum design

(a) Imaging
(b) Beam-shaping

Iterative Fourier algorithm (IFTA)

Image plane

input:

$$A_m(0) = 1$$
$$\psi_m(0) = \text{random}$$

$$U_m^{(k)}, \psi_m^{(k)}$$

$$\phi^{(k)}(\mu, \nu)$$

amplitude adjust. $$U_m^{(k+1)}$$

clipping: $$I(k)_{I} \rightarrow 1$$

DOE plane

$$\mathcal{F}^{-1}$$

$$\mathcal{F}$$

$$U'_m^{(k)}, \psi'_m^{(k)}$$

$$\phi^{(k)}(\mu, \nu)$$

Example: fan-out 9x1

Iterative Fourier Transform Algorithm (IFTA)

Multilevel computer-generated hologram

Simulated annealing

Cost Function $E$
Variable $q$
Probability $P(\Delta E)$
Temperature $T$

Set $T$

Set $q$

Set $q'$

$\Delta E > 0$

$\Delta E = E(q') - E(q)$

$P = \exp(-\Delta E/T)$

$\Delta E \leq 0$

$\alpha = q'$

Accept

Stable?

Yes

Stop

No

Temperature change $T = T'$

$\pi$

$0$

$n$
Diffusers for DUV-lithography: a success story

1994 Feasibility study


Aperture modulated diffusers (AMDs)

Design: IMT
Fabrication: Colibrys
Challenges:
- tolerances scale with wavelengths
- fabrication tolerances
- design to relax fabrication tolerances
Design of an AMD

\[ \Phi(r) = \frac{2\pi r^2}{\lambda} \frac{1}{2f} \]

\[ \sin \theta = \frac{\lambda}{2\pi} \frac{\partial \Phi(r)}{\partial r} = \frac{r}{f} \]

Specification of diffuser

- Flat-top with rectangular shape
- Space invariant design
- Deflection angle of 7 deg at \( \lambda = 248 \text{ nm} \)
  \( \rightarrow \) grating period \( \Lambda = 2 \mu\text{m} \) (mfs = 1 \( \mu\text{m} \))
- High diffraction efficiency > 80 %
- Fabrication of elements in quartz
Diffraction efficiency of binary gratings

\[ \pi \]
\[ \Lambda = 2 \mu m \]

Binary lens \( \eta = 40.5 \% \)
Binary diffuser \( \eta \geq 81.0 \% \)

Far-field of a hexagonal diffuser

![Graph](image-url)
Annular Diffuser

• Input and output planes connected through Fourier transform
  – Each point contributes to all points
• Design based on physical optics
  – Numerical optimization (IFTA)

Comparison between different Solutions

Re-mapping Type Element

• Map transform between input and output planes (point-to-point relation)
• Design based on geometrical optics
  – Analytical (rings, flat-top, gaussian)
  – Inverse ray-tracing

Grating / Diffuser type Element

• Input and output planes connected through Fourier transform
  – Each point contributes to all points
• Design based on physical optics
  – Numerical optimization (IFTA)
**Ideal elements : Re-mapping type**

- Output shape is related to input cell shape. tile-ability problems can appear, or output shape is not completely versatile.
- "lens + slit" effect: oscillations due to diffraction by the cell border are visible

**Ideal elements : Grating type**

- Time and memory consuming design (optimisation can be tedious)
- Noisy intensity distribution
Fabrication errors

- etch depth (binary or multi-level)
- line width (binary or multi-level)
- profile (binary or multi-level)
- mask alignment (multi-level)

Alignment error: Re-mapping type

- Feature size is reduced towards the rim of the DOE
  - Relative alignment error spatially variant
- Point to point relation between DOE and far-field
  - Local influence of the error.
Alignment error: Grating type

- Effective feature size is constant over the whole DOE
  - Alignment error spatially invariant
- No point to point relation between DOE and far-field
  - Global influence of the error.

Summary (diffusers)

Re-mapping type DOE
- Higher-efficiency
- Difficult to generate an arbitrary far-field distribution

Grating type DOE
- Less sensitive to alignment errors
- Nearly any light distribution can be generated
**Limits of paraxial theory**

The interaction of light with structures having geometrical features in the order of the wavelength cannot be described with classical scalar (thin-) diffraction models, but ask for solutions based on Maxwell’s equations.

![Diagram showing thin diffraction theory and rigorous diffraction theory](image)

- **Thin diffraction theory**
  - No polarization
  - No “edge effects”

**Example: rectangular grating**

<table>
<thead>
<tr>
<th></th>
<th>1st order DE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rigorous, $\Lambda = 10 \lambda$</td>
<td>38.796%</td>
</tr>
<tr>
<td>Thin-element</td>
<td>40.528%</td>
</tr>
<tr>
<td>Thin-element+ rejection loss</td>
<td>38.907%</td>
</tr>
</tbody>
</table>

![Graph showing the comparison of 1st order DE](image)
Example blazed grating

\( n_1 = 1 \)
\( n_2 = 1.5 \)
\( d = 2 \lambda \)

Empiric formula for 2x blazed grating

\[ \eta_1 = (1 - p_0) \, \text{sinc}^2 \left( \frac{1}{Q} \right) \left( 1 - \frac{\lambda}{\Lambda p_1} \right) \left( 1 - \frac{\lambda}{\Lambda p_2} \right) \]

- Fresnel reflection loss
\[ p_0 = \left( \frac{n_2 - n_1}{n_2 + n_1} \right)^2 \]

Empiric parameters
\( p_1, p_2 \)
Example \((n_2 = 1.5, n_1 = 1)\)
\( p_1 = -1, p_2 = 1.5 \)

Oblique incidence

The thin element approach predicts that the diffraction efficiency is invariant to the incident angle. Rigorous computations show that this is true only for small incident angles.

Example: binary grating
\( n_2 = 1.5 \)
\( n_1 = 1 \)
\( \Lambda = 4 \lambda \)
\( d = \lambda \)
zero-order grating

**TE-polarization**
\[
\varepsilon_{\text{eff}}^{\text{TE}} = t \varepsilon_1 + (1 - t) \varepsilon_2
\]

**TM-polarization**
\[
\frac{1}{\varepsilon_{\text{eff}}^{\text{TM}}} = \frac{t}{\varepsilon_1} + \frac{(1 - t)}{\varepsilon_2}
\]

**Conclusion: grating classification**

- **Grating**
- **Illumination**
- **\( \lambda \)**
- **\( \Lambda \)**

-  \( \lambda \ll \Lambda \) - thin element domain
-  \( \lambda \gg \Lambda \) - resonance domain
-  \( \lambda \gg \Lambda \) - effective index domain
-  \( \lambda \ll \Lambda \) - rigorous diffraction theory
Artificial index structures

AR coating
\[ \sqrt{n} \]
Substrate
\[ n \]

**Effective medium theory**

**TE-polarization**
\[ \varepsilon_{\text{eff}}^{\text{TE}} = t \varepsilon_1 + (1 - t) \varepsilon_2 \]

**TM-polarization**
\[ \frac{1}{\varepsilon_{\text{eff}}} = \frac{t}{\varepsilon_1} + \frac{1 - t}{\varepsilon_2} \]

Artificial index structures

(zero-order gratings)

- Blazed grating
- Blazed-binary grating
Micro-Optics: system design

- Ray- Tracing & Diffraction
- Non-sequential ray-tracing

Real optical system

pupil function: \( p(x_p, y_p) = |p(x_p, y_p)| \exp[ik \Delta W(x_p, y_p)] \)
**Ray-tracing**

- Plane of incidence
- Refraction: $n_2 \sin I_2 = n_1 \sin I_1$
- Reflection: $I_1 = -I_1'$
- Grating diffraction: $\sin I_2 = \sin I_1 + m \lambda / \Lambda$

**Other interfaces**

Properties can be calculated or measured

---

**Optical path difference (OPD)**

$$OPD = \sum n_i L_i$$

$$\Delta \Phi = \frac{2\pi}{\lambda} \sum n_i L_i$$

Each ray yields values for the amplitude and phase in the exit pupil. The conversion of rays into waves works well for smooth wavefronts.
Illumination light pipe (non-sequential ray-tracing)

- **Goal**
  - flexible illumination by customized extended sources

- **Working principle**
  - Transport of energy
    » TIR guided rays
  - Illumination
    » outcoupled rays

Scattering - possible distributions

## Optics design programs

<table>
<thead>
<tr>
<th>Method</th>
<th>Program</th>
<th>Company</th>
<th>Website</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Optix®</td>
<td>Optenso</td>
<td><a href="http://www.optenso.de">www.optenso.de</a></td>
</tr>
<tr>
<td></td>
<td>ZEMAX®</td>
<td>ZEMAX Development Corporation</td>
<td><a href="http://www.zemax.com">www.zemax.com</a></td>
</tr>
<tr>
<td></td>
<td>WINLENS</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Non-sequential Ray-tracing Programs</td>
<td>ASAP®</td>
<td>Breault Research Organization</td>
<td><a href="http://www.breault.com">www.breault.com</a></td>
</tr>
<tr>
<td></td>
<td>TracePro®</td>
<td>Lambda Research Corporation</td>
<td><a href="http://www.lambdares.com">www.lambdares.com</a></td>
</tr>
<tr>
<td></td>
<td>LightTools®</td>
<td>Optical Research Associates</td>
<td><a href="http://www.opticalres.com">www.opticalres.com</a></td>
</tr>
<tr>
<td></td>
<td>SPEOS®</td>
<td>OPTIS</td>
<td><a href="http://www.optis-world.com">www.optis-world.com</a></td>
</tr>
<tr>
<td></td>
<td>FRED®</td>
<td>Photon Engineering</td>
<td><a href="http://www.photonengr.com">www.photonengr.com</a></td>
</tr>
<tr>
<td></td>
<td>Virtual Lab®</td>
<td>LightTrans</td>
<td><a href="http://www.lighttrans.com">www.lighttrans.com</a></td>
</tr>
<tr>
<td>RCWA</td>
<td>RETICOLO</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>FDTD Solutions™</td>
<td>RSoft Design Group</td>
<td><a href="http://www.rsoftdesign.com">www.rsoftdesign.com</a></td>
</tr>
<tr>
<td></td>
<td>JCMsuite™</td>
<td>JCMwave</td>
<td><a href="http://www.jcmwave.com">www.jcmwave.com</a></td>
</tr>
<tr>
<td></td>
<td>Omnisim™</td>
<td>Photon Design</td>
<td><a href="http://www.photond.com">www.photond.com</a></td>
</tr>
<tr>
<td></td>
<td>OptiFDTD™</td>
<td>Optiwave Systems</td>
<td><a href="http://www.optiwave.com">www.optiwave.com</a></td>
</tr>
<tr>
<td></td>
<td>Microwave Studio®</td>
<td>Computer Simulation Technology</td>
<td><a href="http://www.cat.de">www.cat.de</a></td>
</tr>
<tr>
<td>Finite Elements</td>
<td>FEMlab®</td>
<td>COMSOL</td>
<td><a href="http://www.comsol.com">www.comsol.com</a></td>
</tr>
</tbody>
</table>

Freeware (blue)