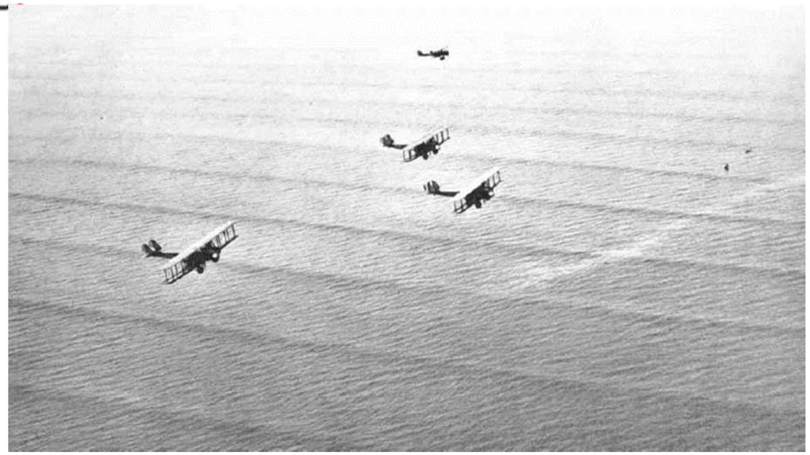
Beam propagation method in X-ray optics simulations

Jacek Krzywinski

SLAC

Catch the Wave(front)



We are talking X-waves
(not X-Rays)

Credits

- ***Jérôme Gaudin -*** European XFEL GmbH
- ***Andrzej Andrejczuk -*** University of Bialystok

Outline

- Introduction
- Paraxial approximation of Helmholtz Equation
- Propagation of coherent X-rays in vacuum and Fourier Optics
- Thin shifter approximation and propagation of coherent X-rays along beamlines
  - Example: simulation of LCLS SXR Instrument performance
- Modeling the interaction of X-rays with optical elements by solving time dependent, 2D Schrödinger equation
  - Examples: mirrors, gratings, and multilayer focusing optics
- Outlook

Introduction

- New X-rays sources produce powerful coherent X-rays (waves)
- Wave propagation, diffraction, and dynamical effects are important for understanding properties of the beam delivered for users
- There are many methods to tackle this problem. One of them is so called Beam Propagation Method (BPM)
- Numerical implementation of BPM is extremely simple, yet the method is very powerful!

Paraxial approximation of Helmholtz Equation in inhomogenous media

Helmholtz Equation for $e^{i\omega t}$ harmonic function

$$(\nabla^2 + k(n(x,y,z))^2)\cdot E(x,y,z) = 0$$

$E(x,y,z) = \psi(x,y,z)\cdot e^{-ikz}$, n – refractive index

Paraxial approximation $k_x{}^2 + k_y{}^2 << k_z{}^2$

or $\left|\frac{\partial^2\psi}{\partial z^2}\right| << \left|2k\frac{\partial\psi}{\partial z}\right|$

Paraxial wave equation

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} - 2ik(n(x,y,z))\frac{\partial\psi}{\partial z} = 0$$

Paraxial approximation of Helmholtz equation in *inhomogeneous* media: Schrödinger equation

for n-1 <<1

$$\frac{\partial\psi(\mathbf{r}_\perp, z)}{\partial z} = \frac{i}{2}[\nabla_\perp\psi(\mathbf{r}_\perp, z) + \boxed{\delta\varepsilon(\mathbf{r}_\perp, z)}\psi(\mathbf{r}_\perp, z)]$$

Difference between dielectric constant of vacuum and the media

Length unit $k = \frac{2\pi}{\lambda} = 1.$

$$\frac{\partial\psi}{\partial z} = iH\psi$$

Identical to 2D, time dependent Schrödinger equation

$$H = \frac{1}{2}\nabla_\perp^2 + \frac{1}{2}\delta\varepsilon(\mathbf{r}_\perp, z)$$

solution

$$\psi(z) = \psi(0)e^{iHz}$$

Propagation in vacuum - Fourier Optics

$$\frac{\partial \psi}{\partial z} = iH\psi$$

$$H = \frac{1}{2}\nabla_{\perp}^{2} + \cancel{\frac{1}{2}\delta\varepsilon(\mathbf{r}_{\perp}, z)}$$

$$\psi(\mathbf{r}_{\perp}, z) = \psi(\mathbf{r}_{\perp}, 0)e^{iHz}$$

Fourier transform

$$\psi(\mathbf{p}, \mathbf{0}) = \mathcal{F}\mathbf{t}[\psi(\mathbf{r}_{\perp}, \mathbf{0})]$$

$$\psi(\mathbf{p}, L) = \psi(\mathbf{p}, 0)e^{i\frac{\mathbf{p^2}}{2}L}$$

$$\boxed{\psi(\mathbf{r}_{\perp}, L) = \mathcal{F}t^{-1}[\psi(\mathbf{p}, 0)e^{i\frac{\mathbf{p^2}}{2}L}]}$$

Spectral method

Could be implemented using **FFT!**

Implementation of the spectral method in Matlab is extremely simple (8 lines of code)

```
function [psi_r] =f_free_prop_barcelona_scpectr(dx,Z,psi0)
%  Spectral/Fourier Wavefront  Propagation Algorithm
% ==Inputs==
% psi0 = Input field in the space domain
% dx, space step of the psi0 matrix
% Z = propagation distance
% ==Outputs==
%psi_r = Output field in the space domain
% written by Jacek Krzywinski
%=============================================================
% Propagation , 0 to Z
%=============================================================

[Mx,My] = size(ut0);
dkx=2*pi/(dx*Mx); dky=2*pi/(dy*My);
nx =((1:Mx)-Mx/2); ny=((1:My)-My/2);
[kx,ky] = meshgrid(nx*dkx,ny*dky);
k2=kx.^2+ky.^2;
%======================
% FFT of the input field and
% shift  - moving the zero-frequency component to the center of the array
%======================
psift =         (fft(fftshift(psi0)));
%==================================
% Propagation
%=================================
psi_k=psift.*exp(Z.*(-1i/2).*k2);
%==================================
% Shifted Inverse Fourier transform
%=================================
psi_r= :        (ifft2(fftshift(psi_k)));
```

Propagation in vacuum – Fourier Optics

$$\psi(\mathbf{p}, L) = \psi(\mathbf{p}, 0) e^{i\frac{\mathbf{p^2}}{2}L}$$

Convolution theorem

$$\psi(\mathbf{r}_{2\perp}, L) = \frac{2\pi i}{L} \int \psi(\mathbf{r}_{\perp}, 0) e^{\frac{i}{2L}(\mathbf{r}_{2\perp} - \mathbf{r}_{\perp})^2} d(\mathbf{r}_{\perp})$$

Fresnel-Kirchhoff integral

Far zone

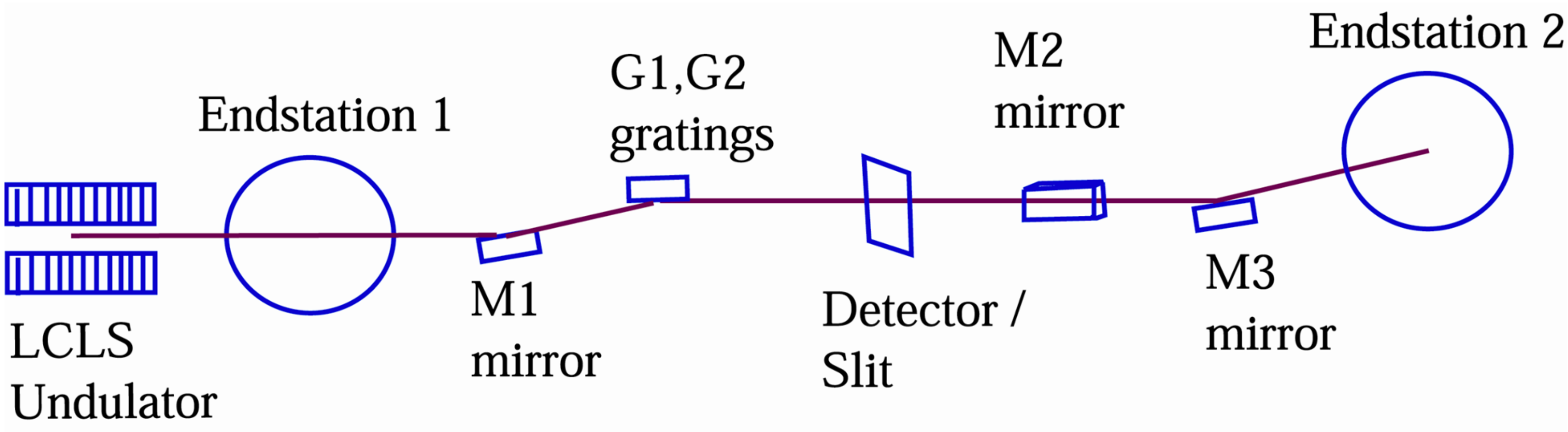
Could be implemented using **FFT (12 lines of code)!**

Spectral method

$$\psi(\mathbf{r}_{\perp}, L) = \mathcal{F}t^{-1}[\psi(\mathbf{p}, 0) e^{i\frac{\mathbf{p^2}}{2}L}]$$

Near zone

LCLS SXR Instrument



	Type	Coating and blank material	Dimensions (mm)	Clear Aperture (mm	Radius (m)	Incidence angle(°)	Grating period order	Distance from source (m)
Enstation 1								124
M1	Spherical mirror	B_4C-coated silicon	250 x 50	185 x 10	1049	89.20	-	125.1
G1, G2	Plane VLS grating	B_4C -coated silicon	220 x 50	180 x 34	∞	88.56-89.03	1/100, 1/200 -1	125.4
Detector/ Slit								132.9
M2	Bent Elliptical mirror	B_4C-coated silicon	250 x 30	205 x 10	281.6	89.20	-	137.4
M3	Bent Elliptical mirror	B_4C-coated silicon	250 x 30	120 x 10	164.8	89.20	-	137.9
Endstation 2								139.4

P. Heimann et. al., Rev. Sci. Instrum. **82, 093104 (2011)**

Thin phase shifter approximation

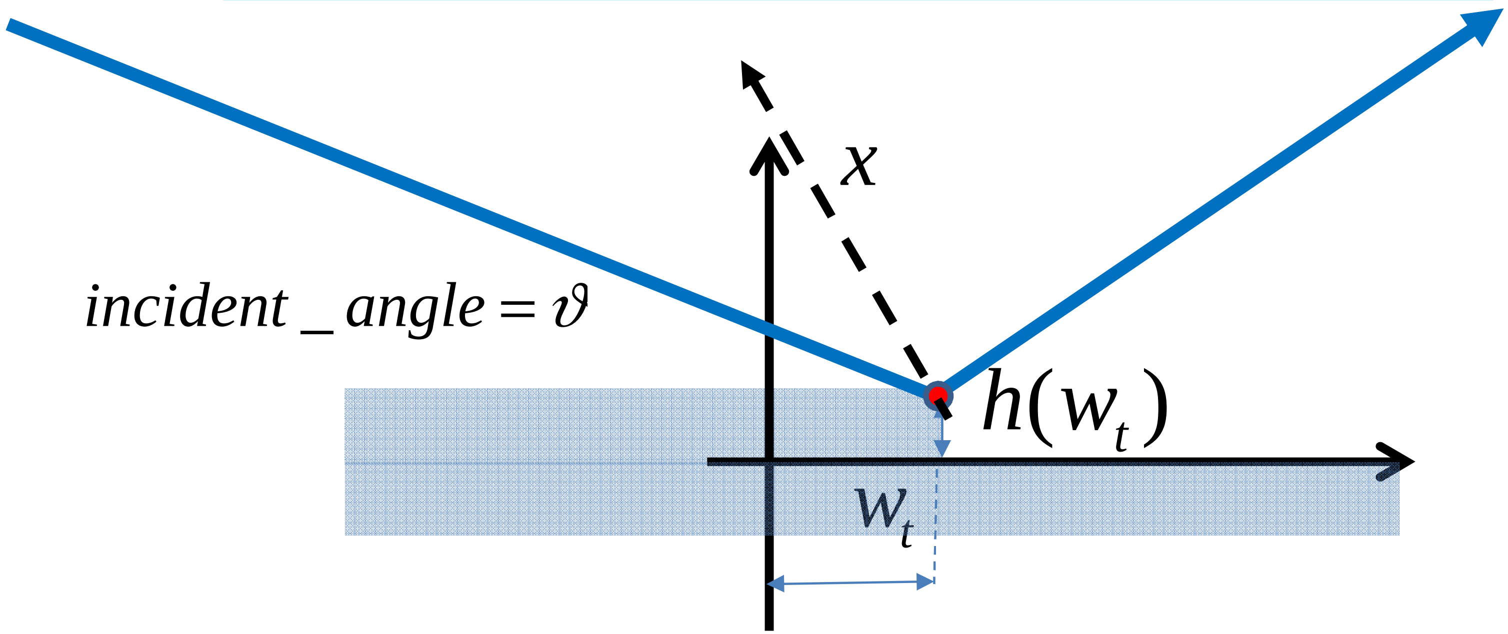
$$\Delta\varphi(\vec{r}) = \frac{2\pi}{\lambda}\cdot OPD$$

$$\psi'(\mathbf{r}_\perp, 0) = \psi(\mathbf{r}_\perp, 0)e^{i\Delta\varphi(\mathbf{r}_\perp)}$$

For the small WF curvature case

$$OPD \approx 2\cdot\vartheta\cdot h(w_t)$$

$$\mathbf{r}_\perp = [x, y] = [\varphi\cdot w_t, w_s]$$

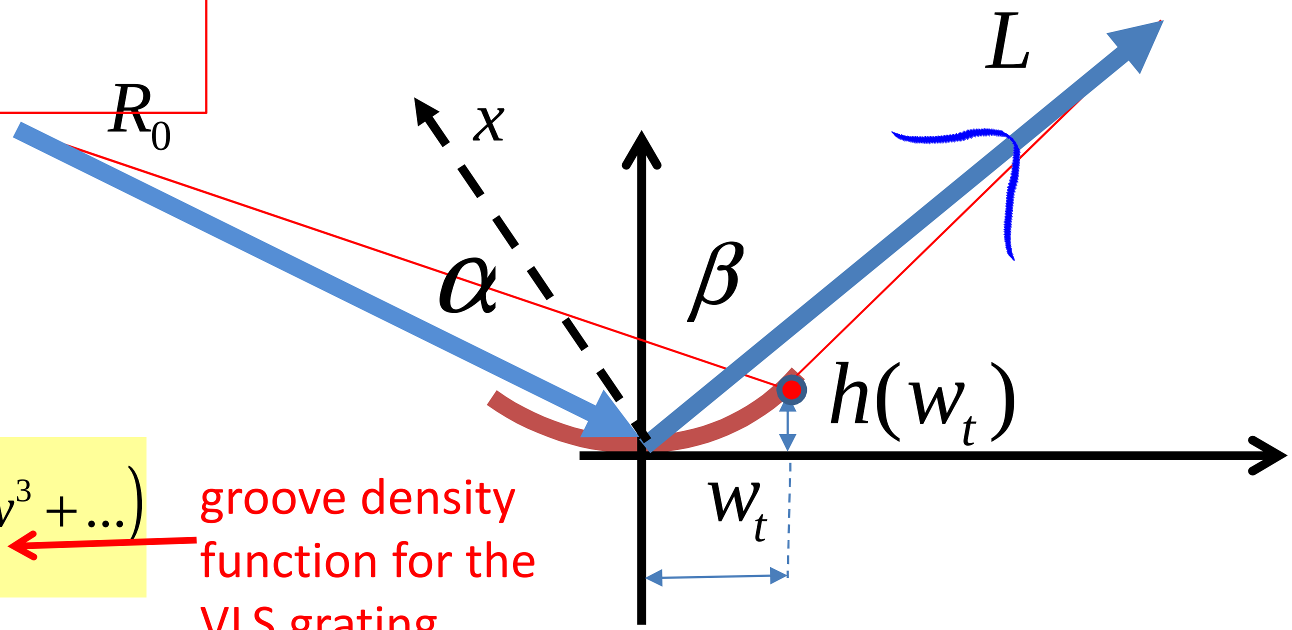


Thin phase shifter approximation

$$\boxed{\psi'(\mathbf{r}_\perp,0)=\psi(\mathbf{r}_\perp,0)e^{i\Delta\varphi(\mathbf{r}_\perp)}}$$

$$\Delta\varphi(\vec{r})=\frac{2\pi}{\lambda}\left\{n(\vec{w})+R_0+L-\left[\begin{array}{l}\sqrt{(R_0\cos(\alpha)-h(\vec{w}))^2+(R_0\sin(\alpha)+w)^2}+\\ \sqrt{(L\cos(\beta)-h(\vec{w}))^2+(L\sin(\beta)+w)^2}\end{array}\right]\right\}$$

R_0, L are the average radiuses of curvatures of incident and scattered wavefronts , β is derived from the grating equation

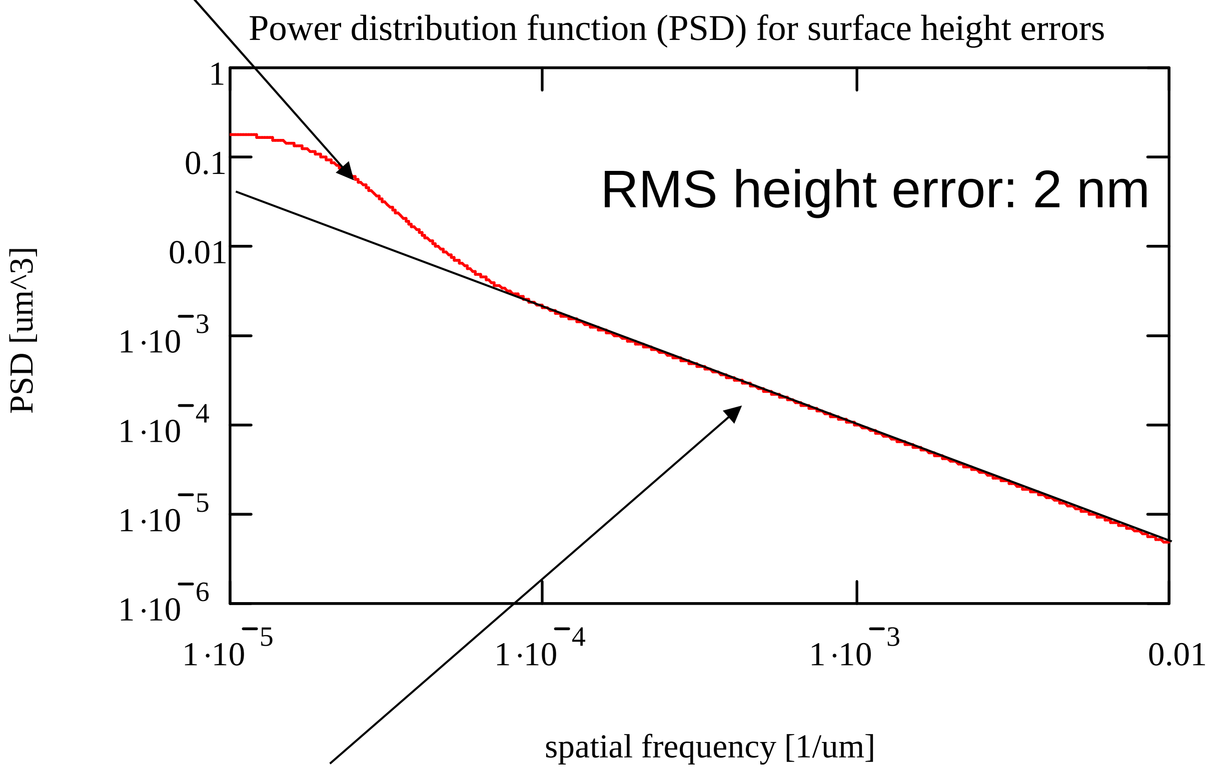


$$n(w)=\frac{1}{\sigma_0}\left(w+n_2w^2+n_3w^3+\ldots\right)$$

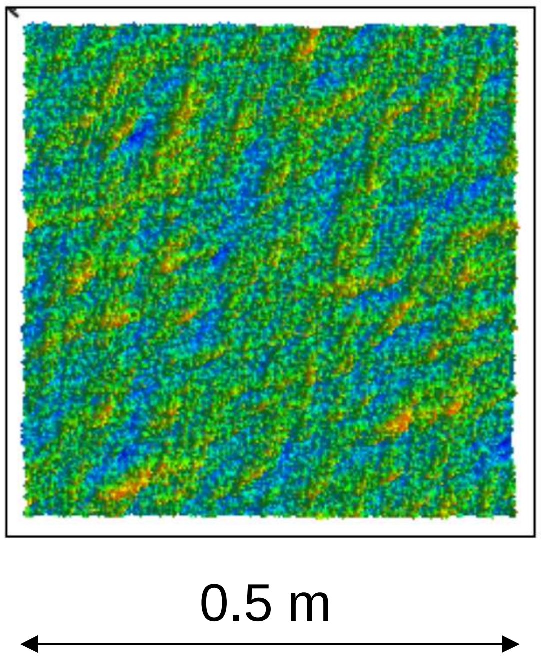
groove density function for the VLS grating

Model of surface roughness

Model for figure errors is based on mirror specification (height, slope error)

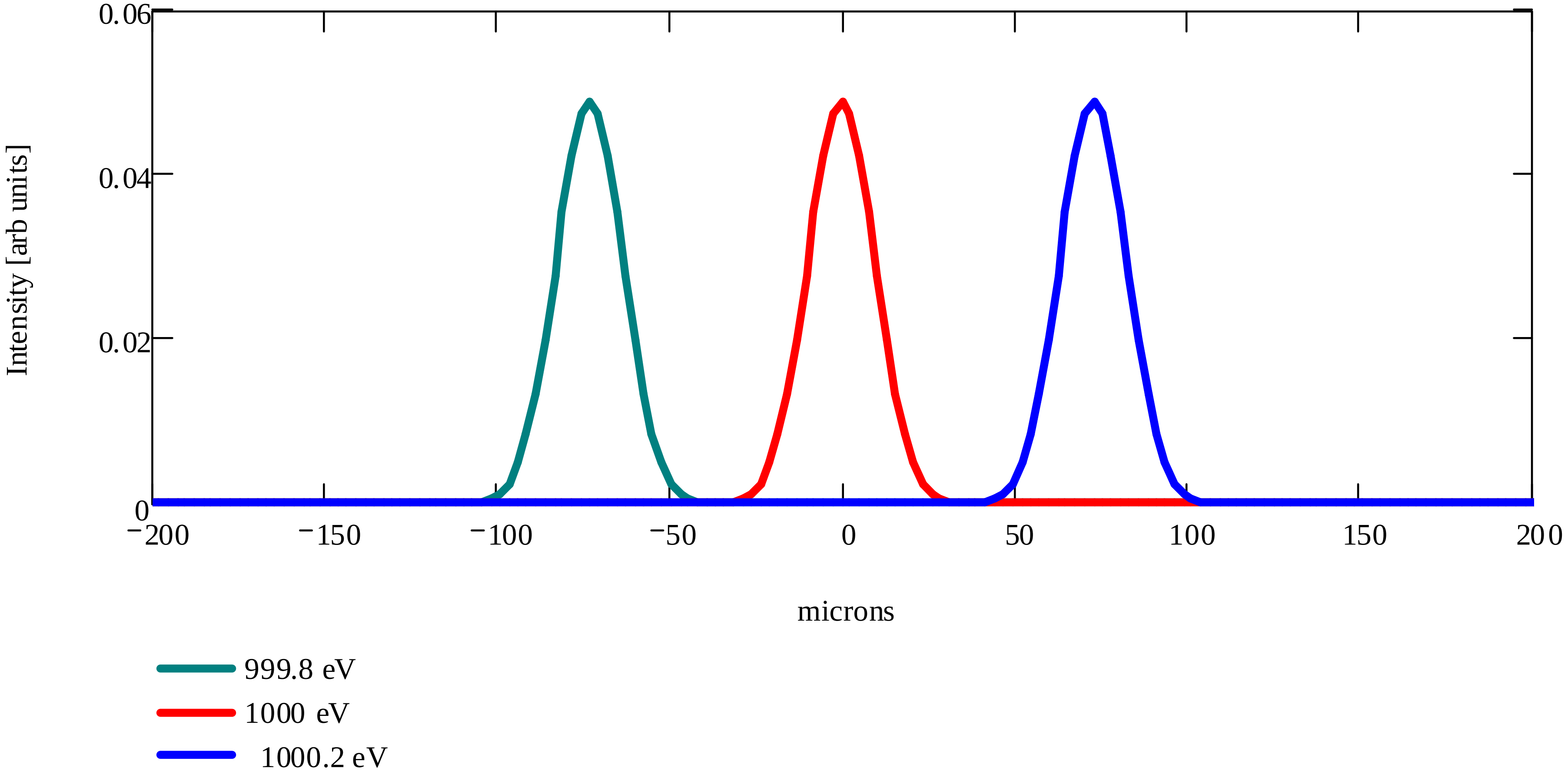


Fractal model for mid and high frequency errors, based on mirror specifications

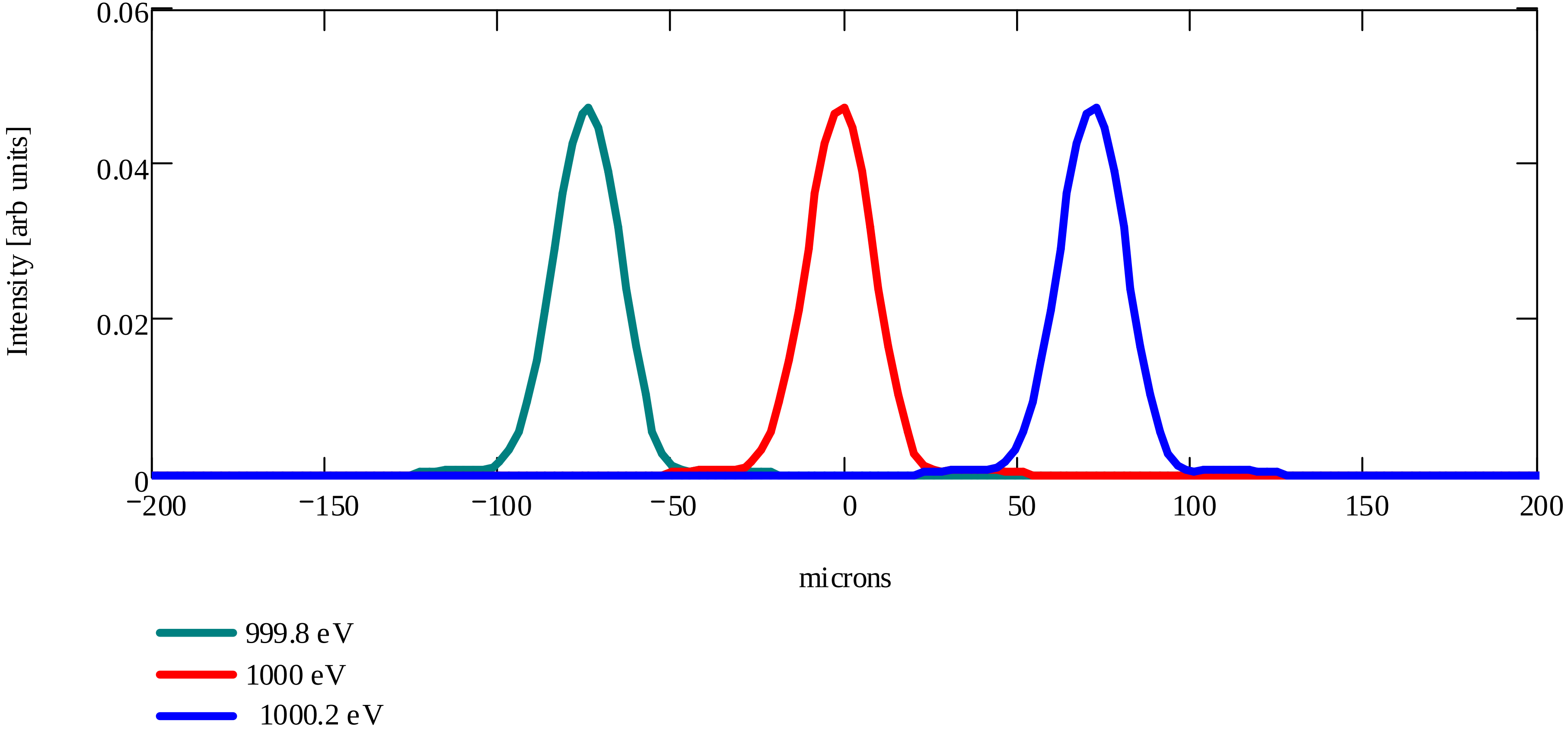


Generated surface errors

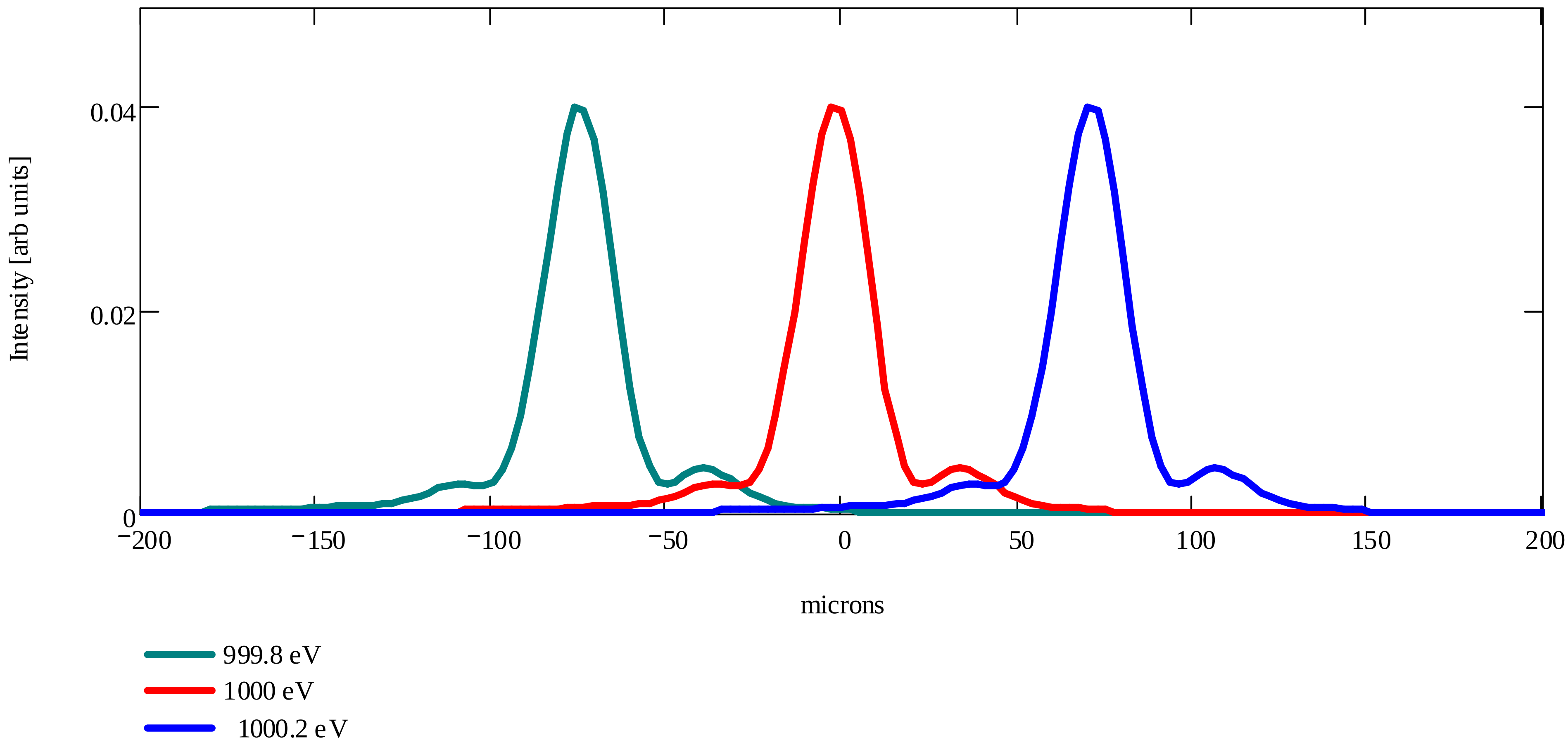
At slit position, no surface errors



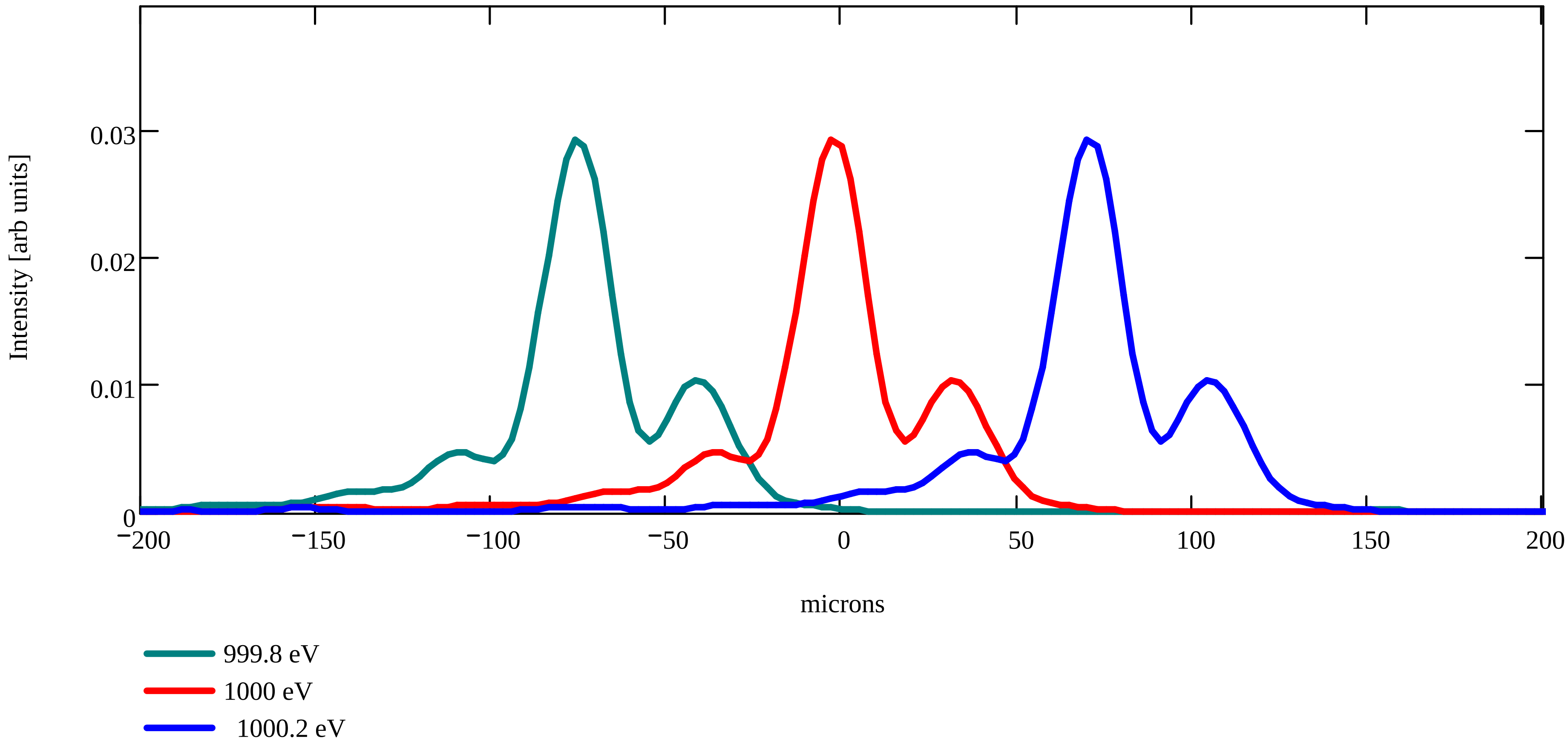
At slit position, 1 nm, 0.25 urad rms surface errors



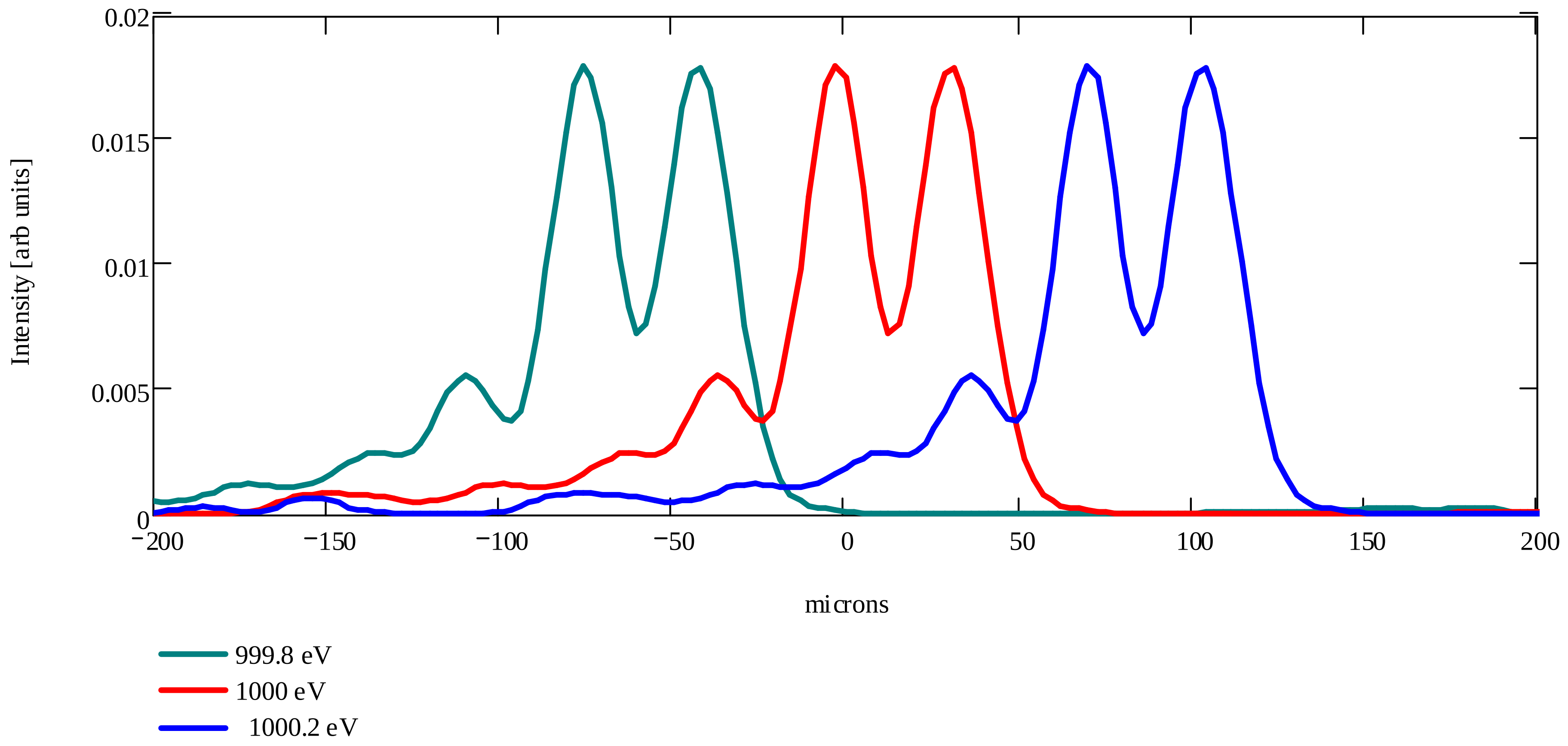
At slit position, 2 nm, 0.25 urad rms surface errors



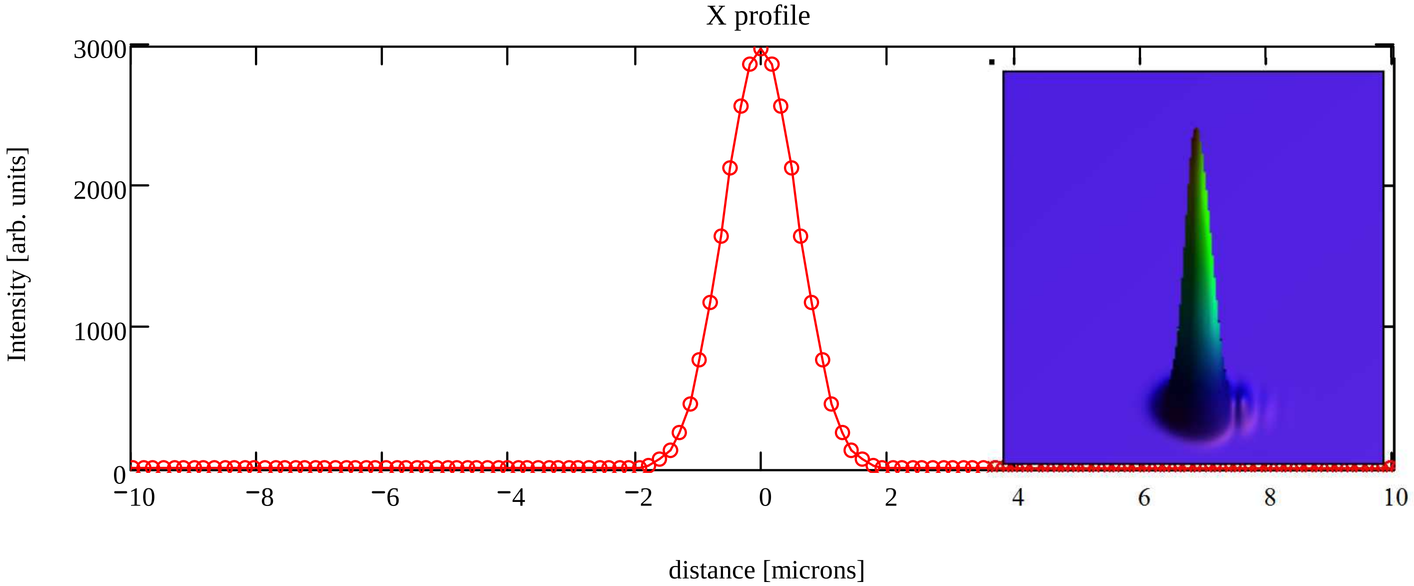
At slit position, 3 nm, 0.25 urad rms surface errors

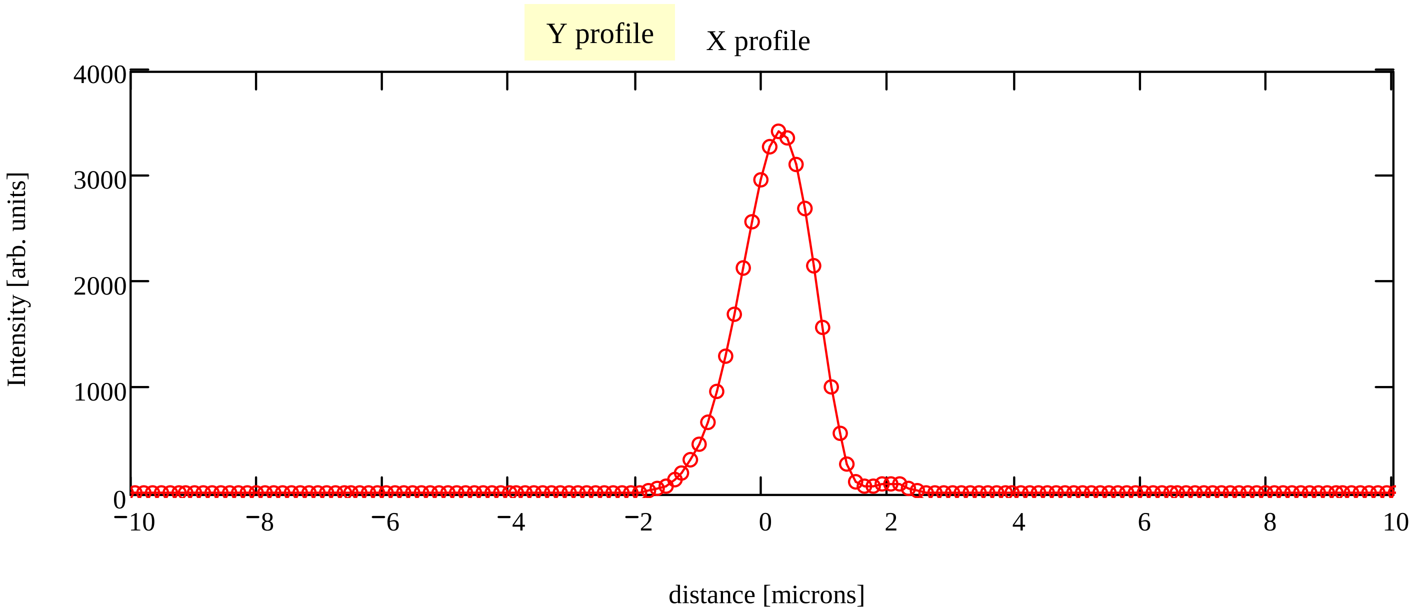


At slit position, 4 nm, 0.25 urad rms surface errors

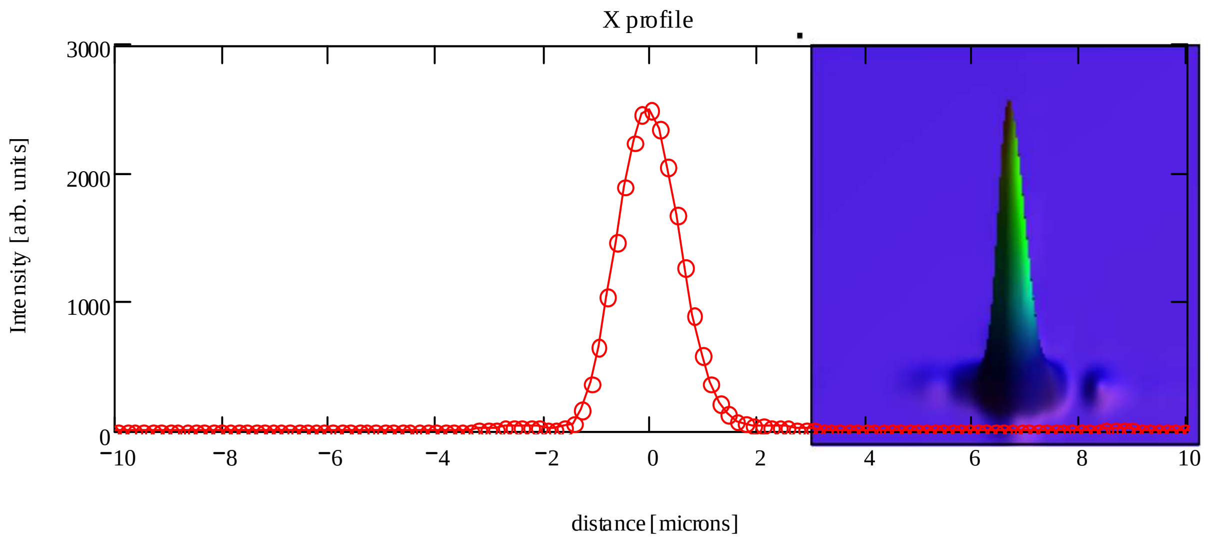


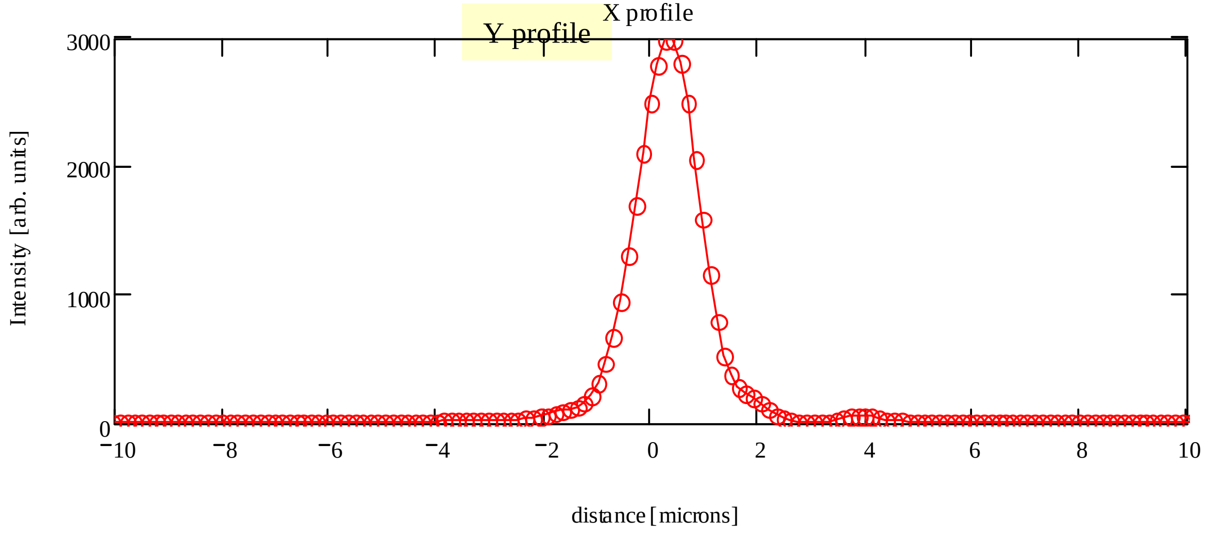
At end station position, no surface errors, pink beam, at the focus



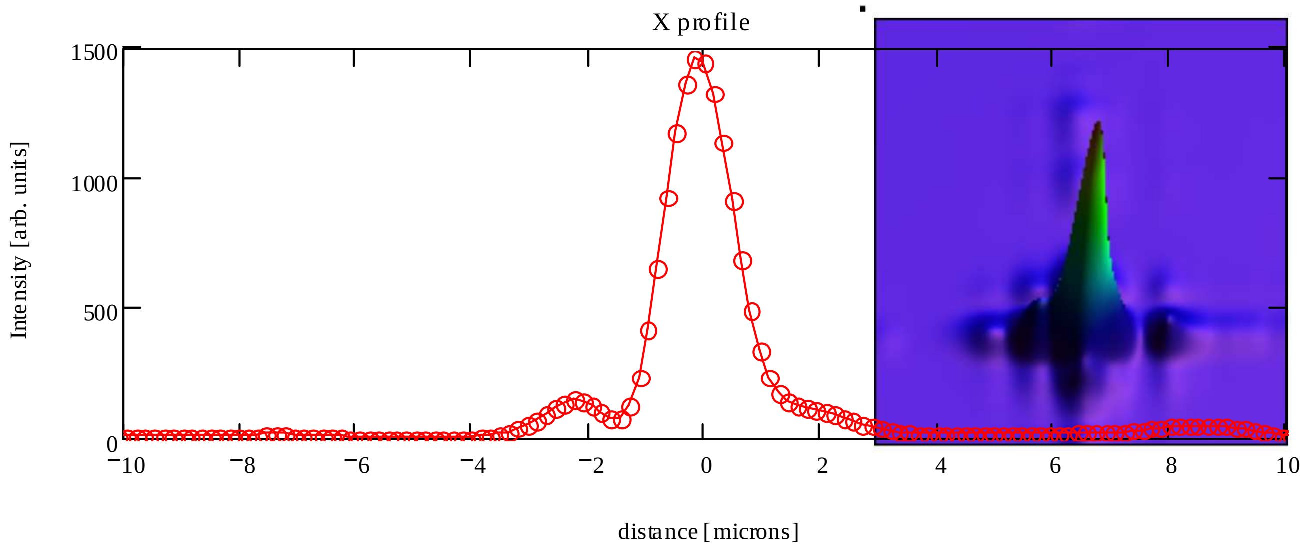


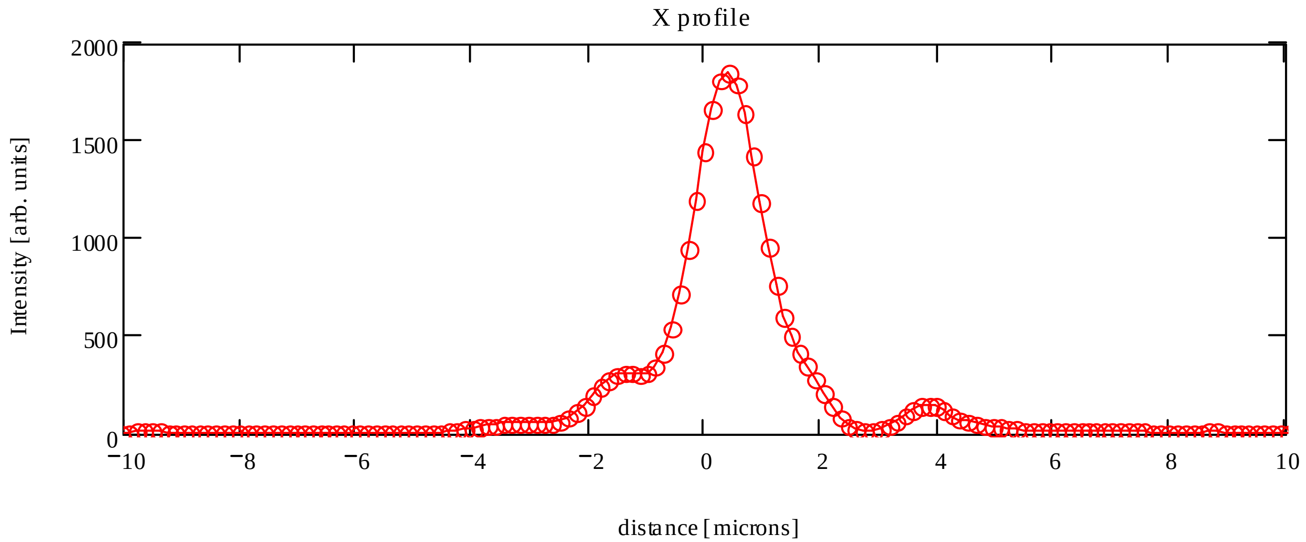
At end station position, 1 nm, 0.25 urad rms surface errors, pink beam, at the focus



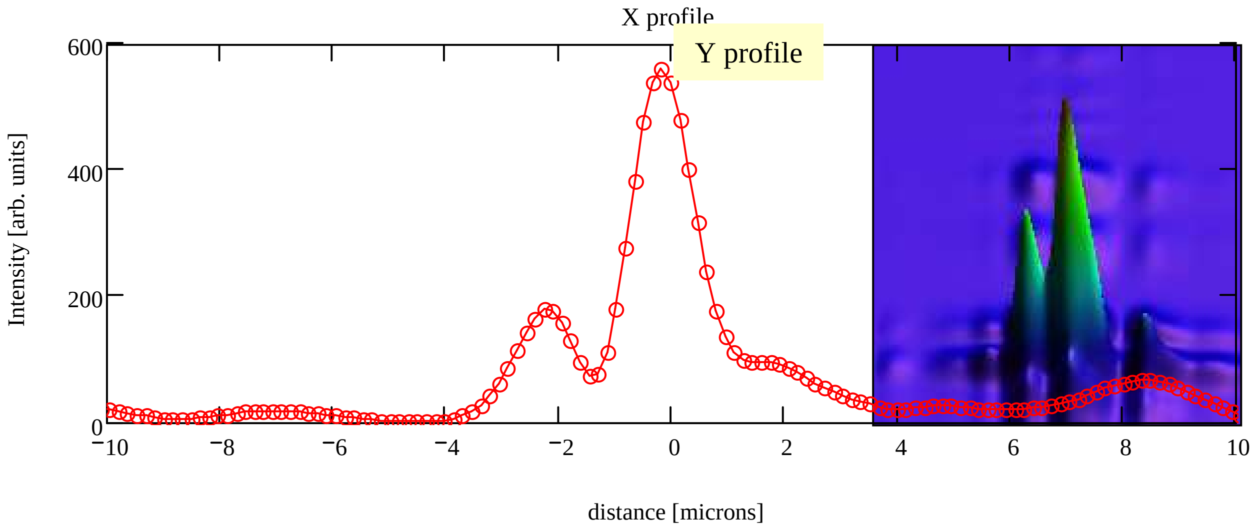


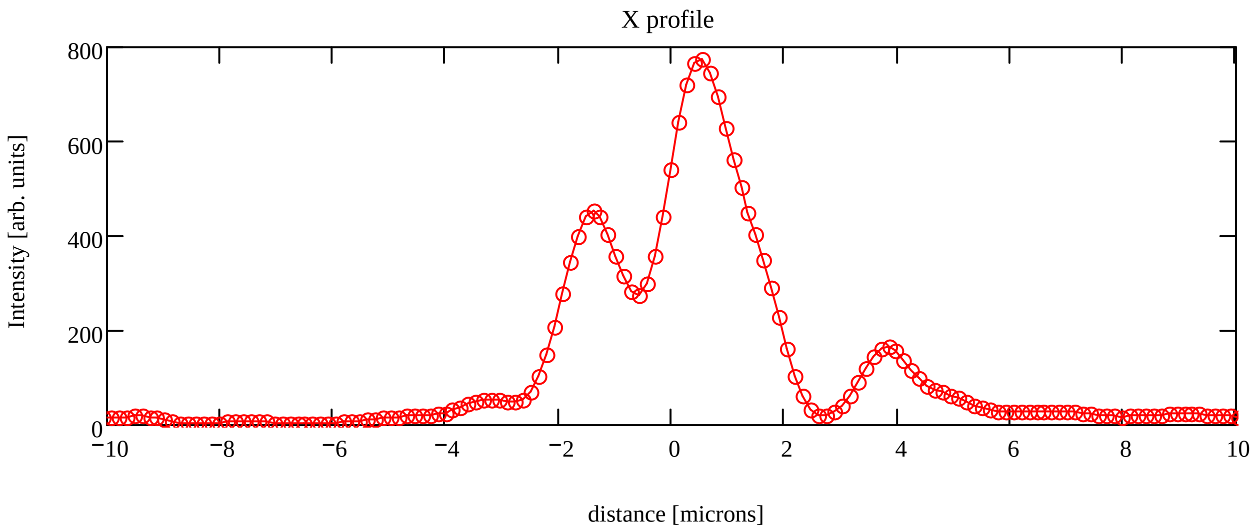
At end station position, 2 nm, 0.25 urad rms surface errors, pink beam, at the focus



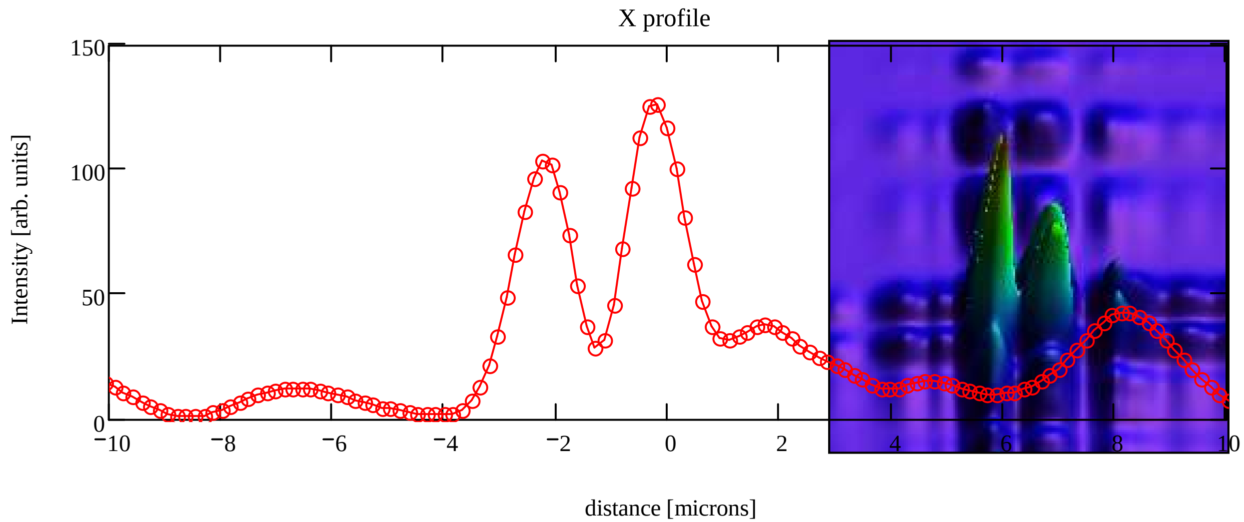


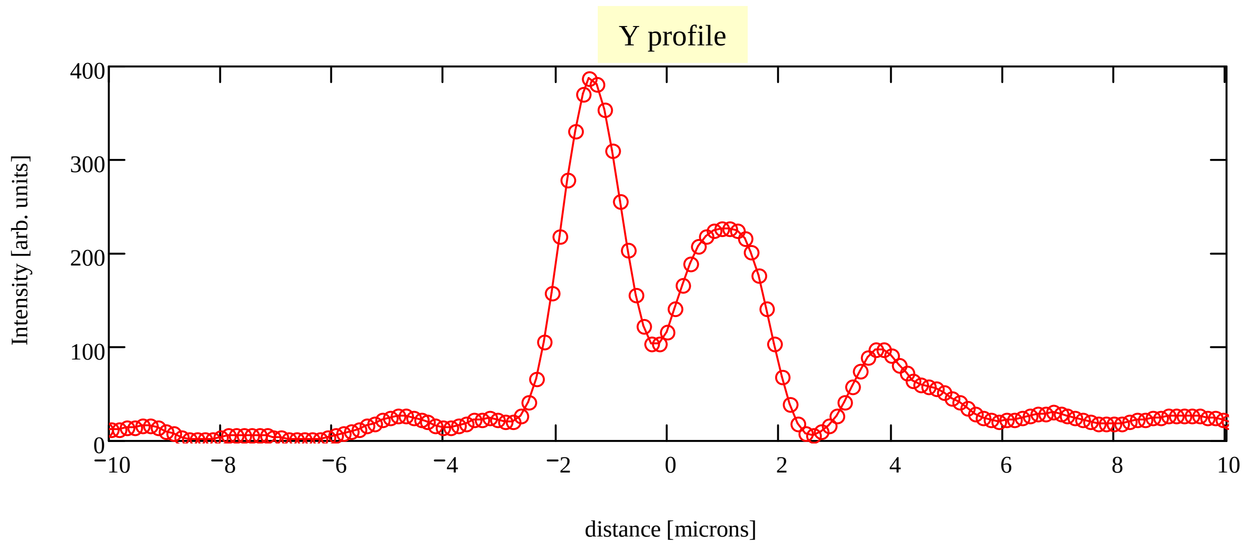
At end station position, 3 nm, 0.25 urad rms surface errors, pink beam, at the focus





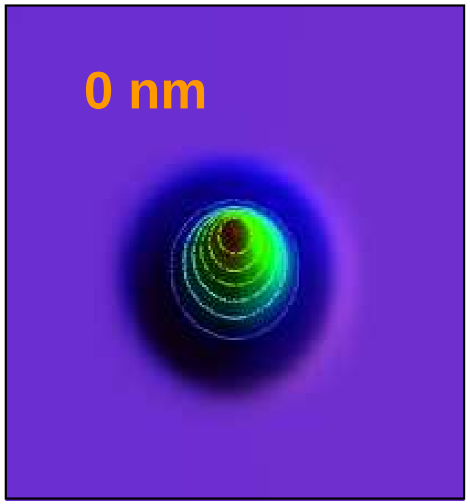
At end station position, 4 nm, 0.25 urad rms surface errors, pink beam, at the focus

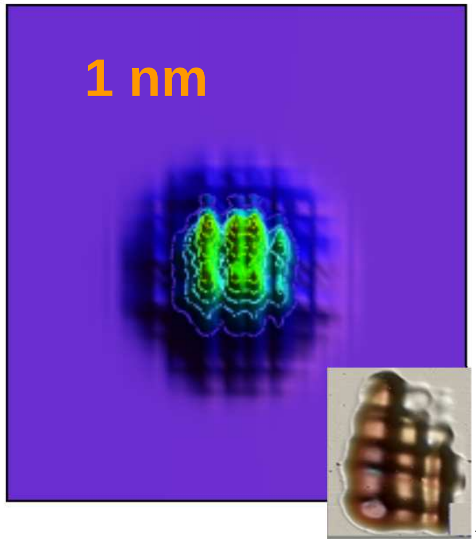




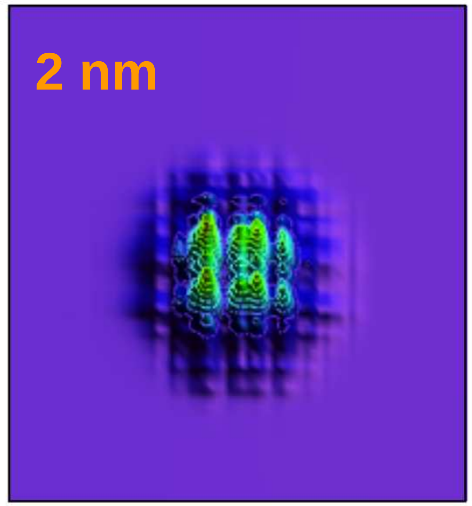
At end station position, 0.25 urad rms surface errors, pink beam, 10 cm behind the focus

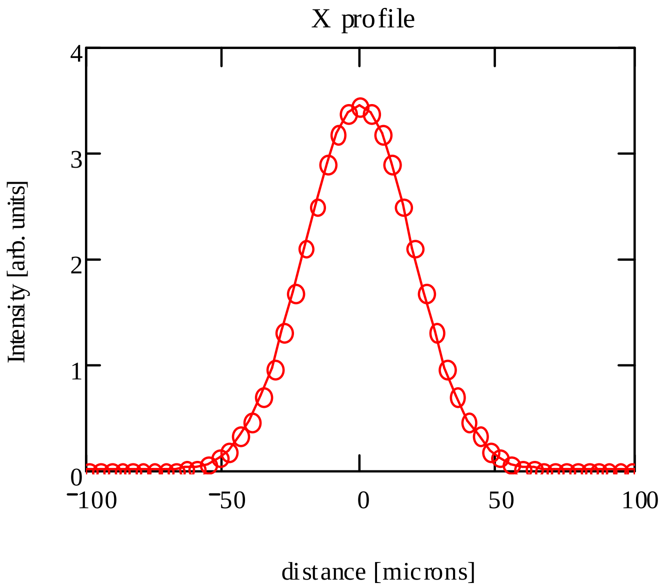
Figure error (rms):

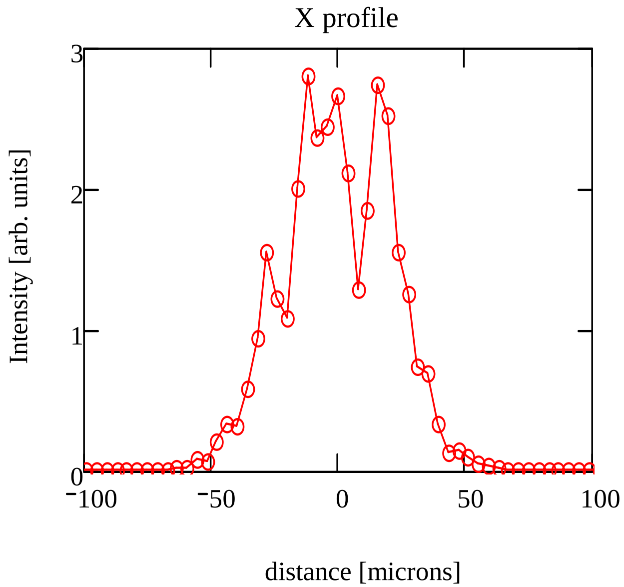


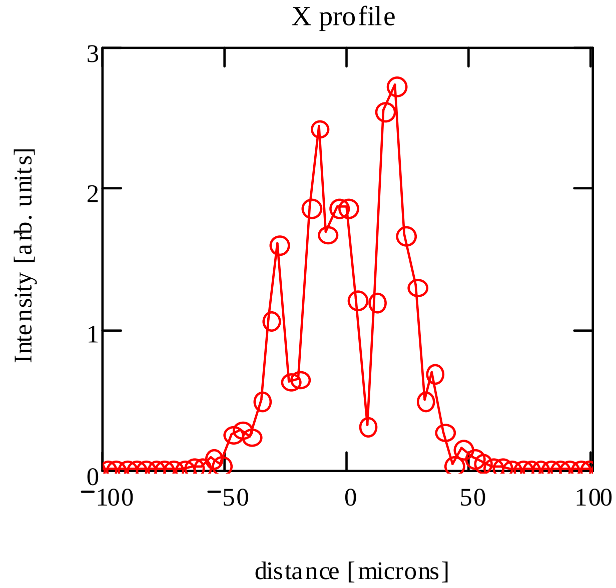


AMO out of focus imprint









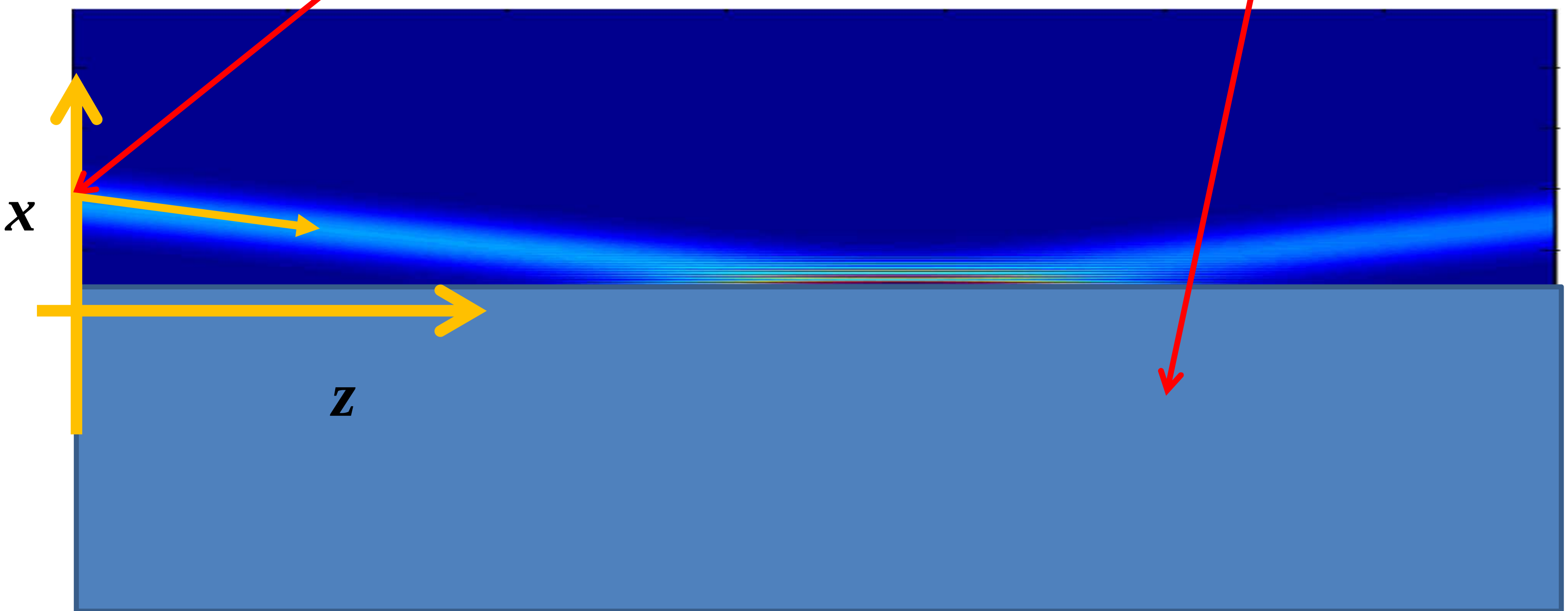
Propagation in inhomogeneous media:

Flat mirror

$$\frac{\partial \psi}{\partial z} = iH\psi$$

$$H = \frac{1}{2}\nabla_{\perp} + \frac{1}{2}\delta\varepsilon(\mathbf{r}_{\perp}, z)$$

$$\psi(\mathbf{r}_{\perp}, z) = \psi(\mathbf{r}_{\perp}, 0)e^{iHz}$$



Split operator method (14 lines of code)

For operators which do not commute :

$$e^{(P+V)} \neq e^{P} e^{V}$$

but for sufficiently small dz this relation is nearly fulfilled

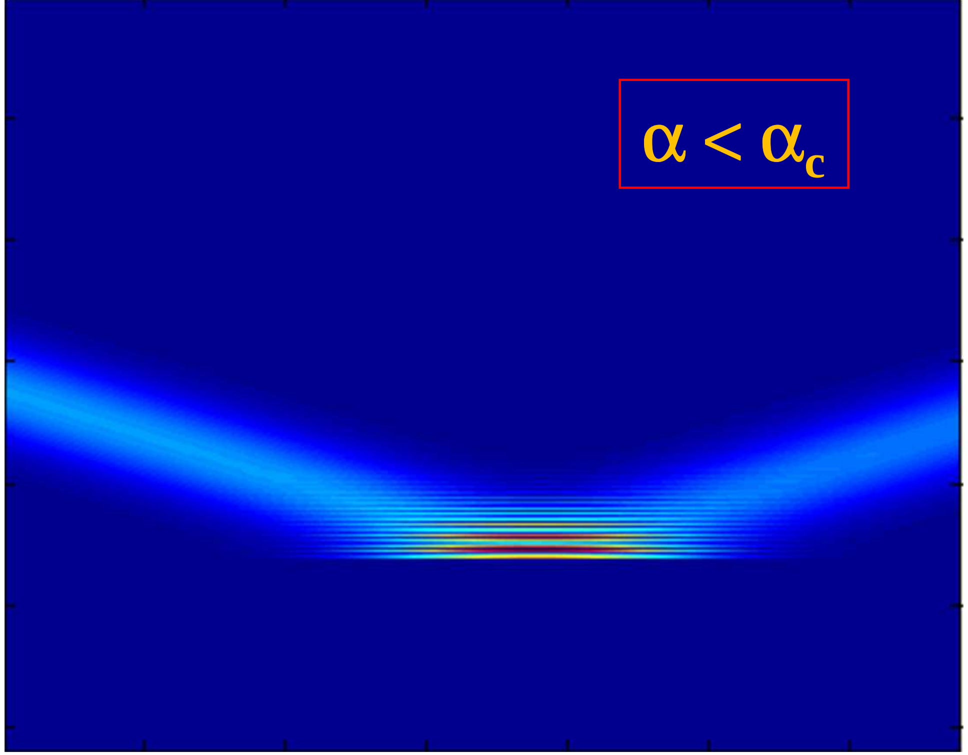
$$e^{(P+V)dz} \approx e^{Pdz} e^{Vdz}$$

and

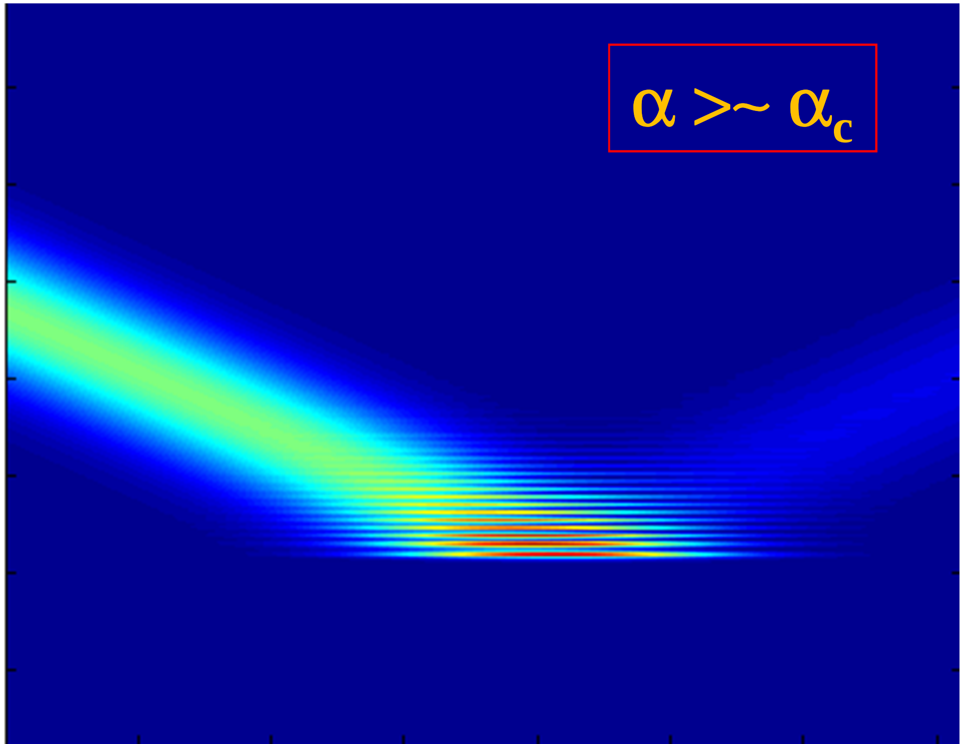
$$\boxed{\psi(x,z+dz) \approx e^{\frac{i}{2}\nabla^2 dz} e^{\frac{i}{2}\delta\varepsilon(x,z)dz} \psi(x,z)}$$

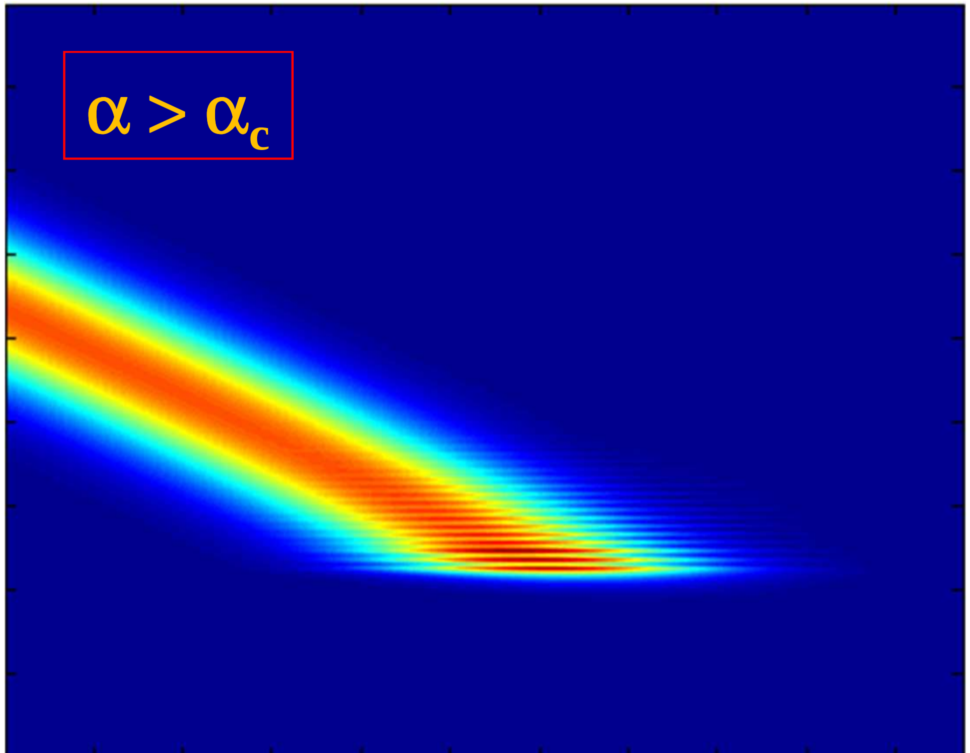
Split operator method (14 lines of code)

```
function [U_out]=f_prop_grat_prof(conversion_from_SI_units,...
    M,X0,delta_eps1,delta_eps2,h_C,x,kx,U_in,dz,prof_ext)
 %'kinetic' part of the Hamiltonian in momentum space
Hk=exp(-i/2*kx.^2*dz);
 %Fourier transform of the field in the space domain
G=fftshift(fft(U_in));
% the main loop begins here
for k = 1:M
G1=G.*Hk;
U_out1=ifft(ifftshift(G1));
  %definition of the dielectric constant distribution
    X1=-prof_ext(k);
    log_a1=x>X0+X1;
    log_b1= X0+X1>=x & x>=X0+X1-h_C;
    delta_eps=log_a1*delta_eps1+log_b1*delta_eps2;
% 'potential energy' part of the Hamiltonian
Hz=exp(i/2*(delta_eps)*dz);
U_out = U_out1.*Dz;
G= fftshift(fft(U_out));
end
```



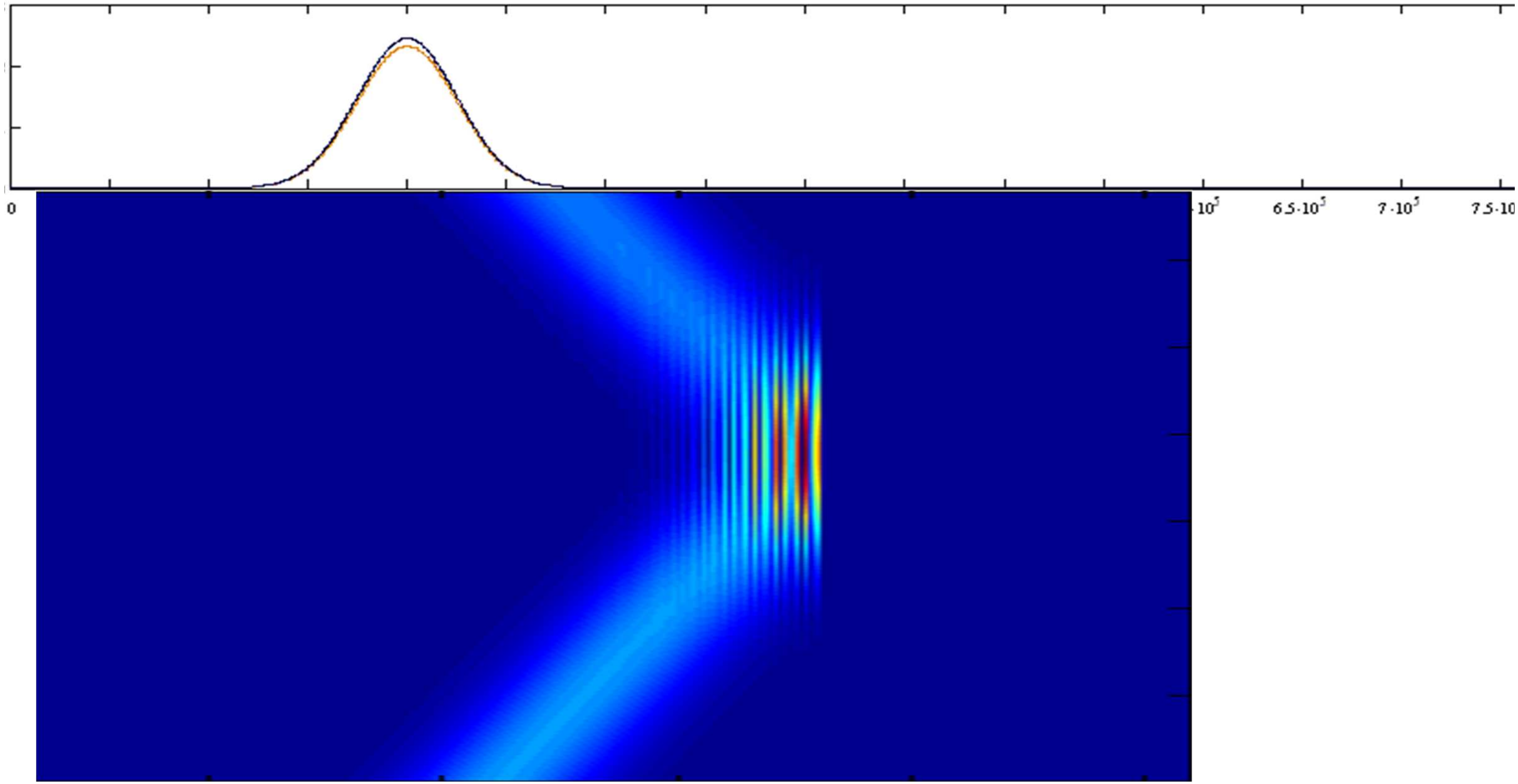
50 nm a-C layer on Si substrate, Gaussian source, Photon Energy 290 eV





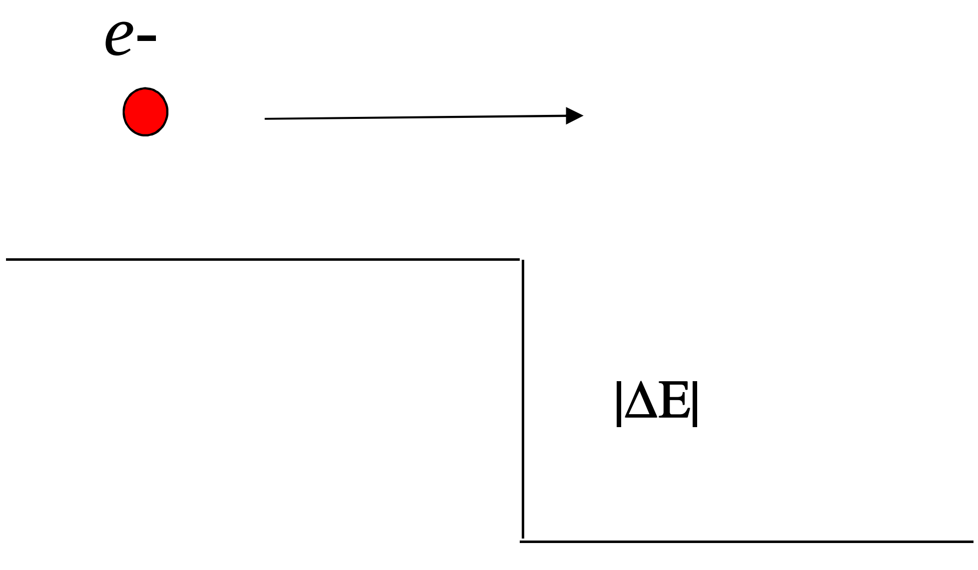
$\boxed{\alpha < \alpha_c}$

rows(mac2) = 217



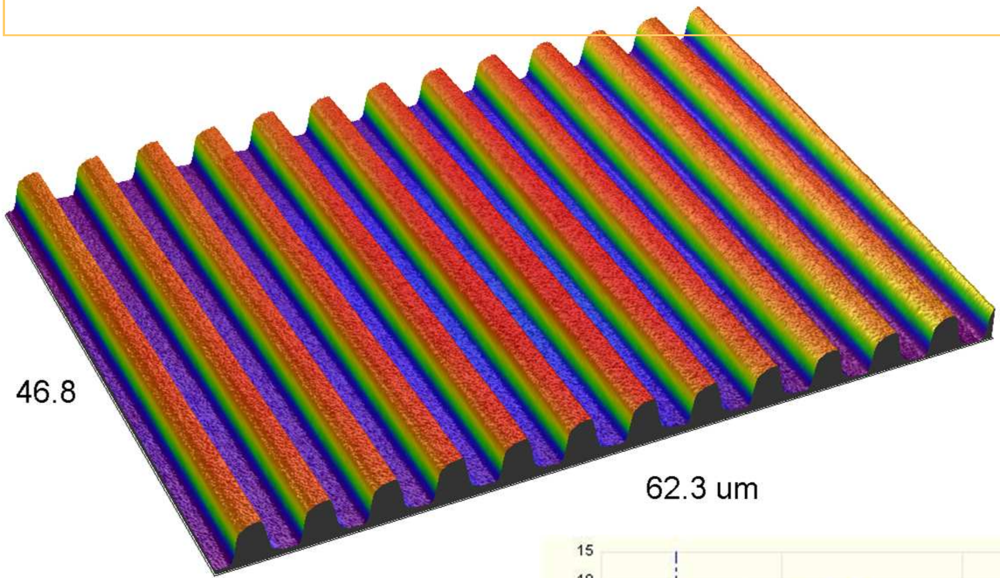
Analogy in QM

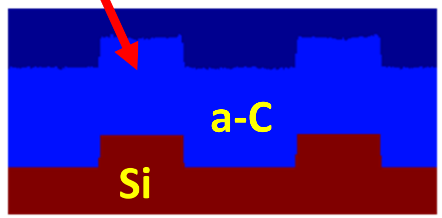
- The same problem as inelastic electron scattering by a potential barrier
- Incident angle corresponds to electron’s kinetic energy



Grating

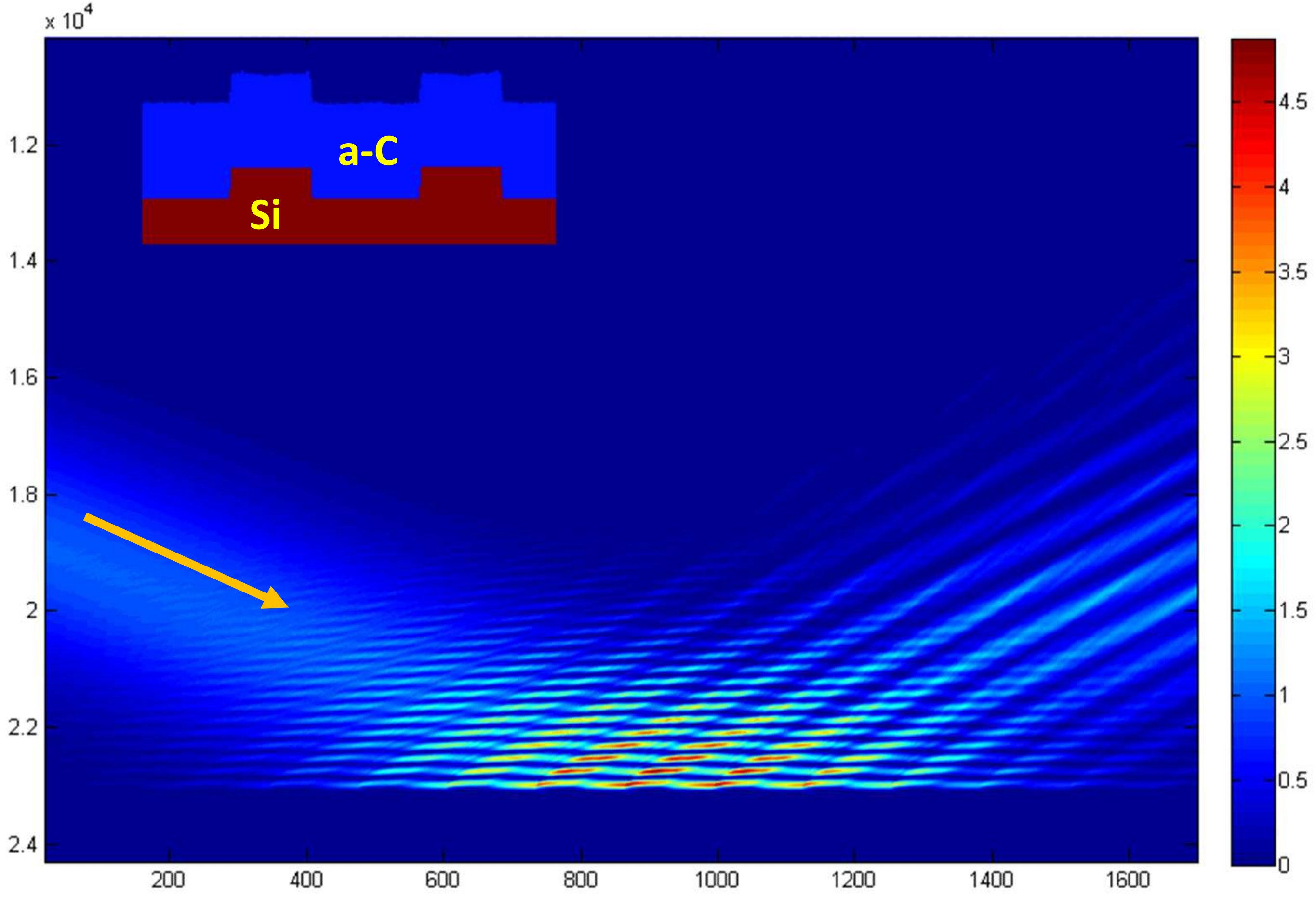
$$\frac{\partial \psi(\mathbf{r}_\perp, z)}{\partial z} = \frac{i}{2}\left[\nabla_\perp \psi(\mathbf{r}_\perp, z) + \boxed{\delta\varepsilon(\mathbf{r}_\perp, z)}\,\psi(\mathbf{r}_\perp, z)\right]$$





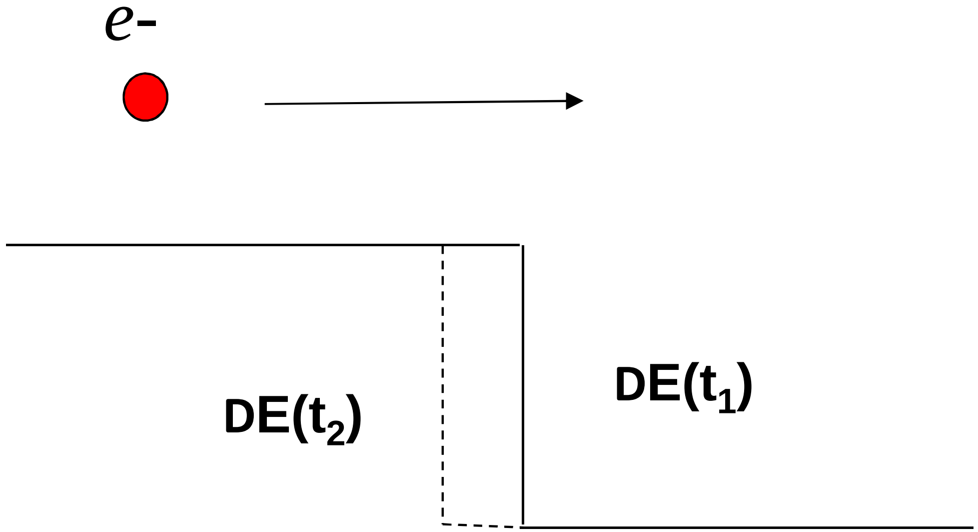
50 nm a-C layer on Si substrate

Simulated field distribution



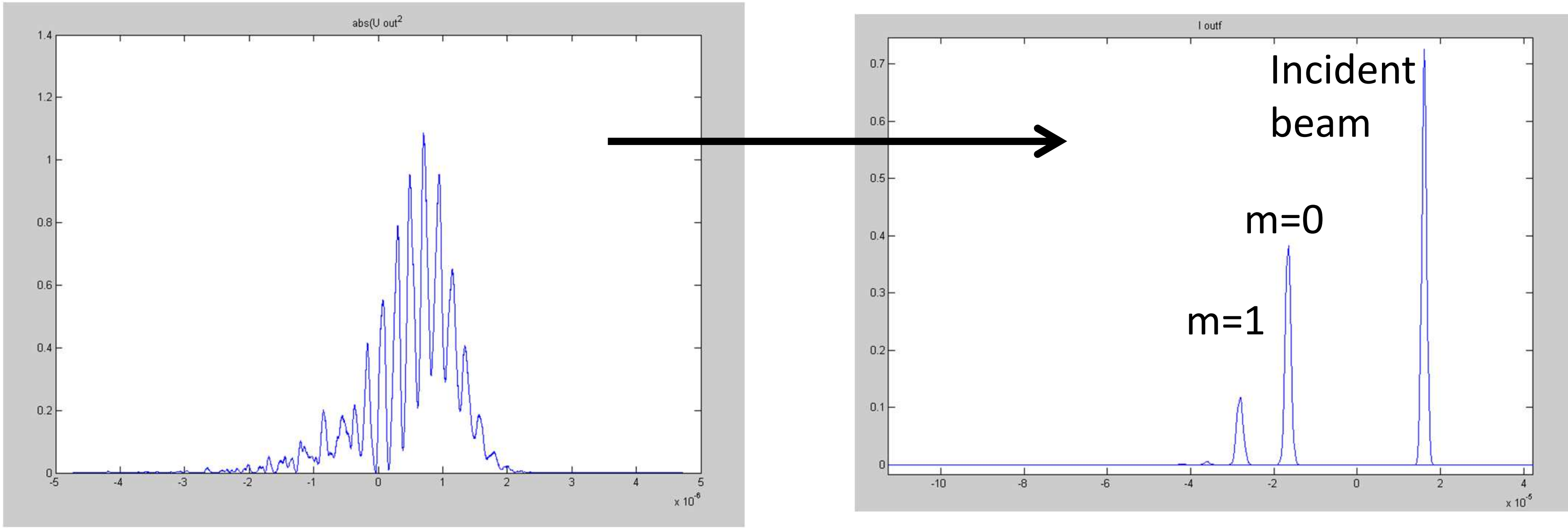
Rough surface - analogy in QM

- The same problem as electron and the potential barrier
- Incident angle corresponds to electron's kinetic energy
- Position of the barrier depends on time



Efficiency of the grating

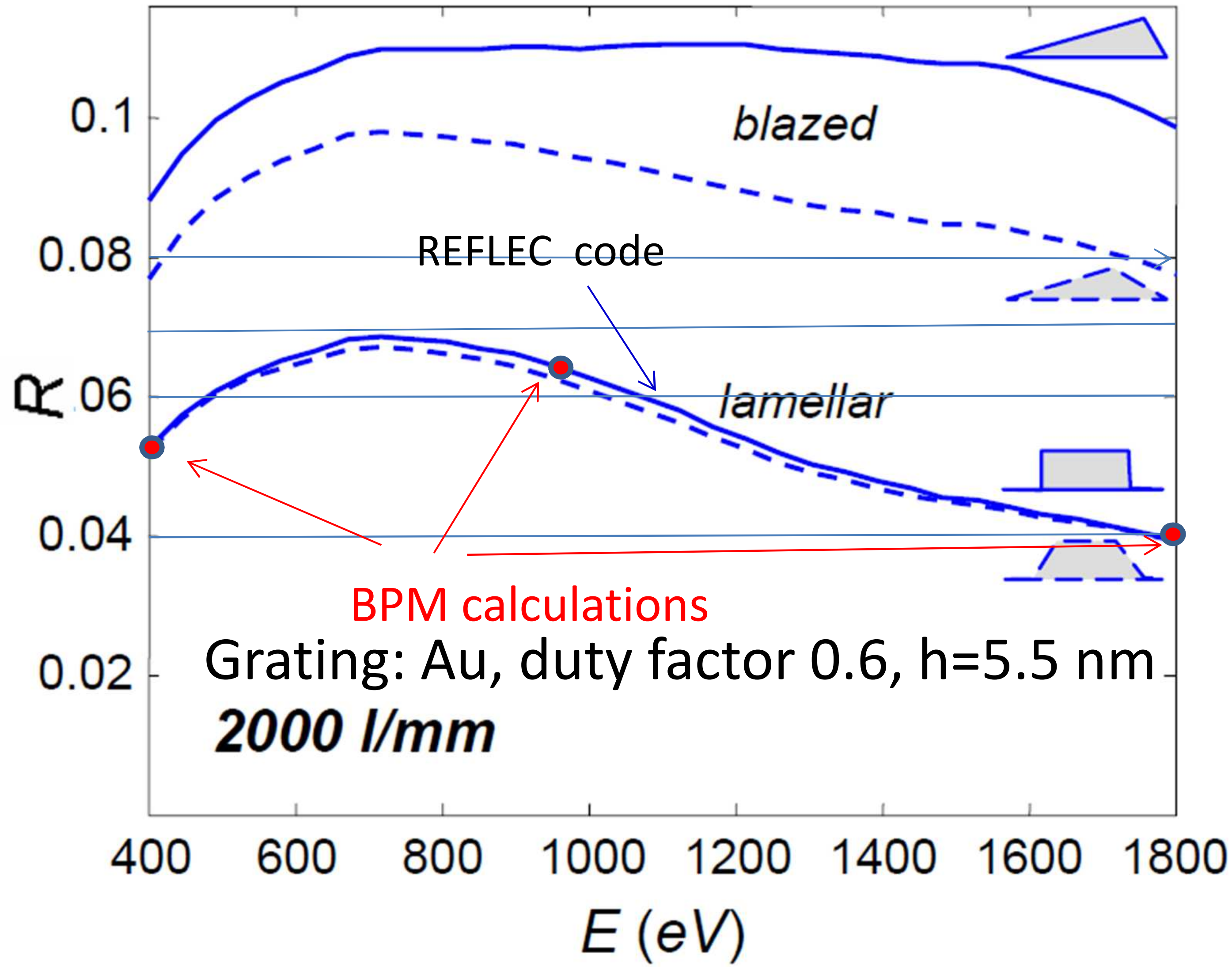
Propagation to far field (FFT)



Diffraction orders

Benchmarking the BPM code v.s. REFLEC[1,2] code

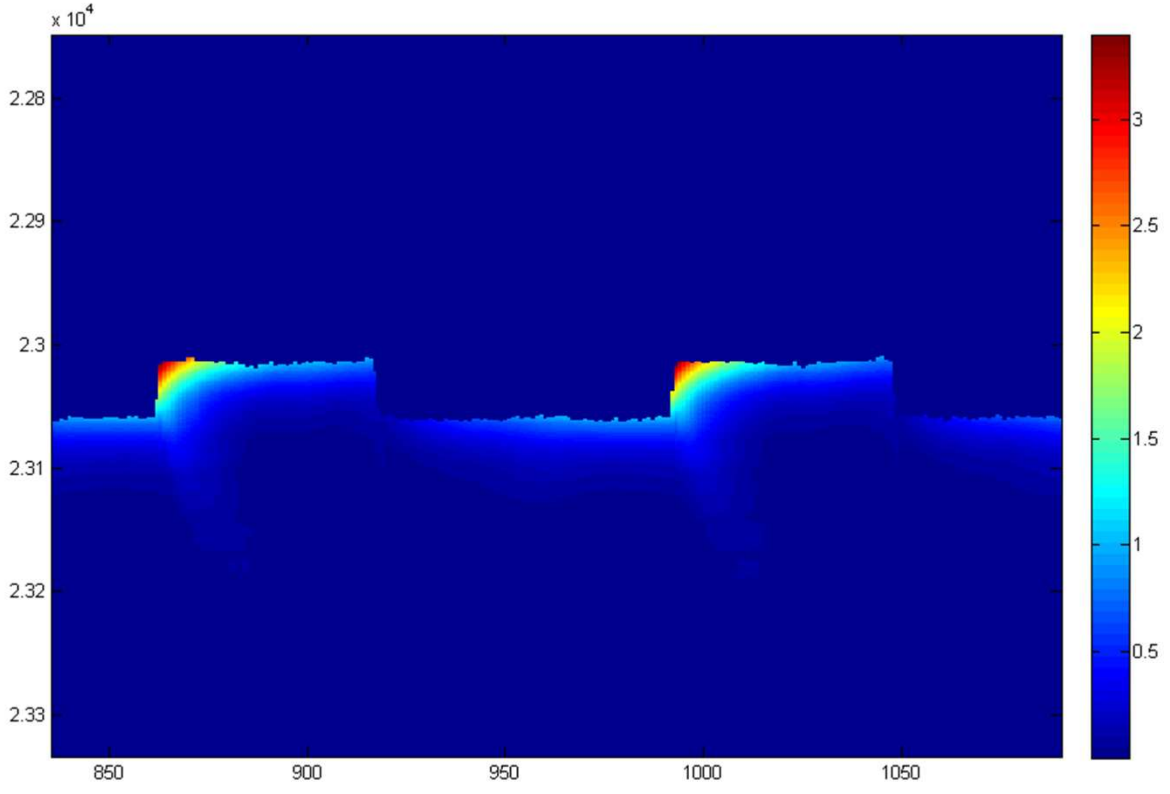
[1] VN Strocov et.al. High-resolution soft-X-ray beamline ADRESS at Swiss Light Source..
http://arxiv.org/pdf/0911.2598



[2] *REFLEC, a program to calculate VUV/X-ray optical elements and synchrotron radiation beamline, F. Schaefers, D. Abramsohn and M. Krumrey (BESSY, 2002). The code is based on the method described in M. Nevière, P. Vincent and D. Maystre, Appl. Optics* ***17 (1978) 843***

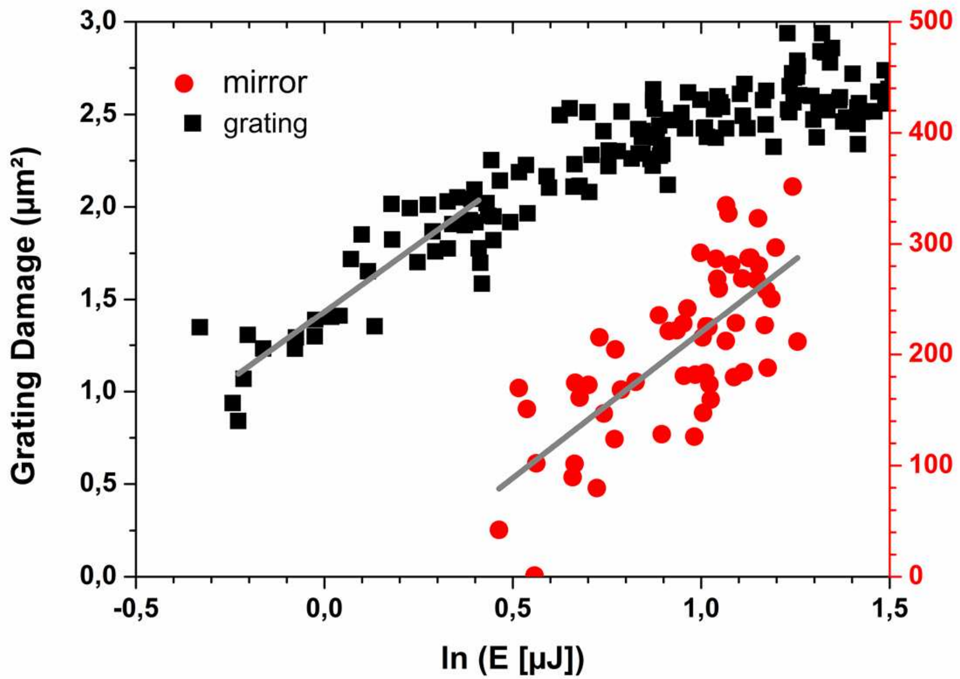
Absorbed power density, 2 deg grazing incidence angle

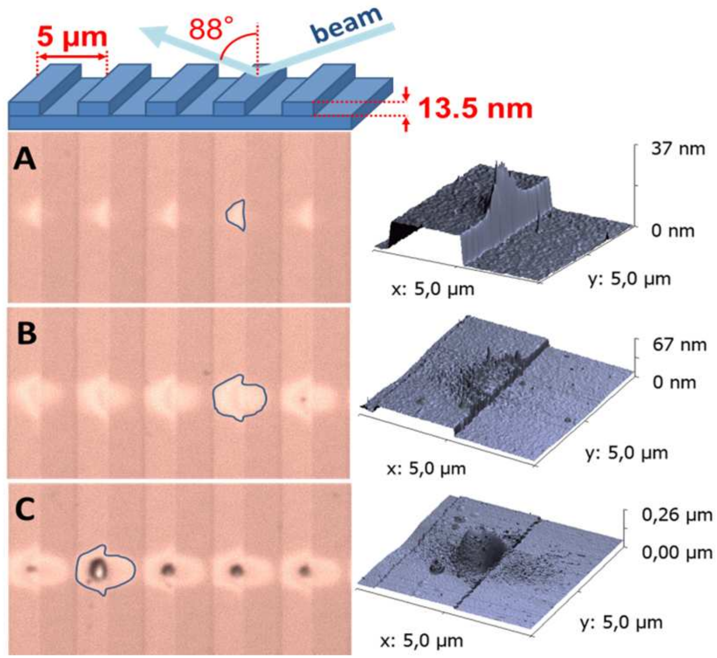
The simulation shows that the specific field distribution at the surface leads to an enhancement of the absorbed energy at the edge of the laminar grating structure.

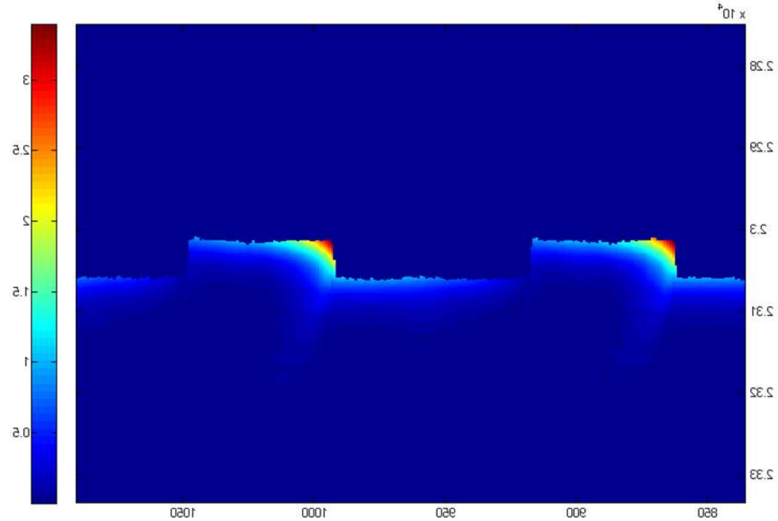


Interestingly, micro-roughness does not increase the maximum of absorbed energy by more than few percent

Damage experiment at FLASH





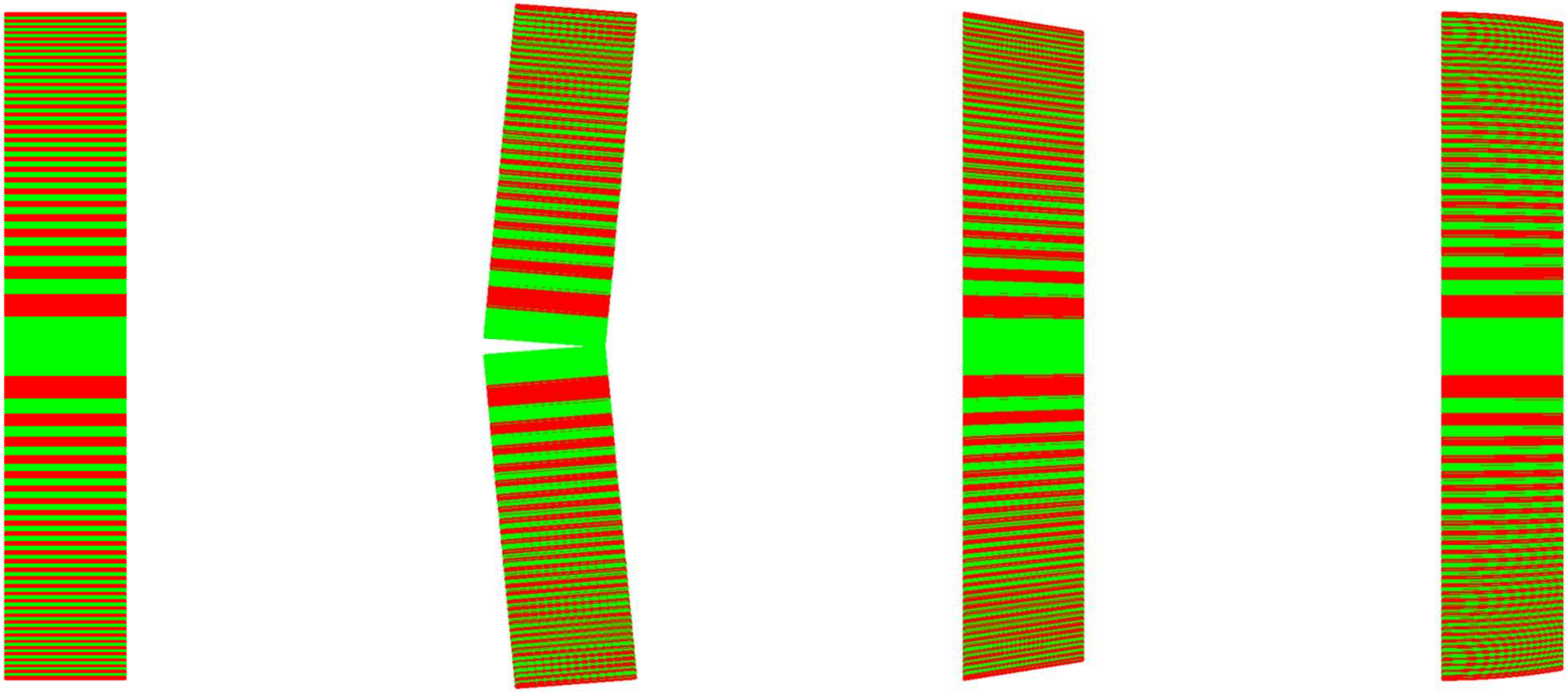


The model provides a good qualitative and quantitative description of the experimental results. The measured and simulated damage threshold is 3.5 times lower than obtained for the flat surface.

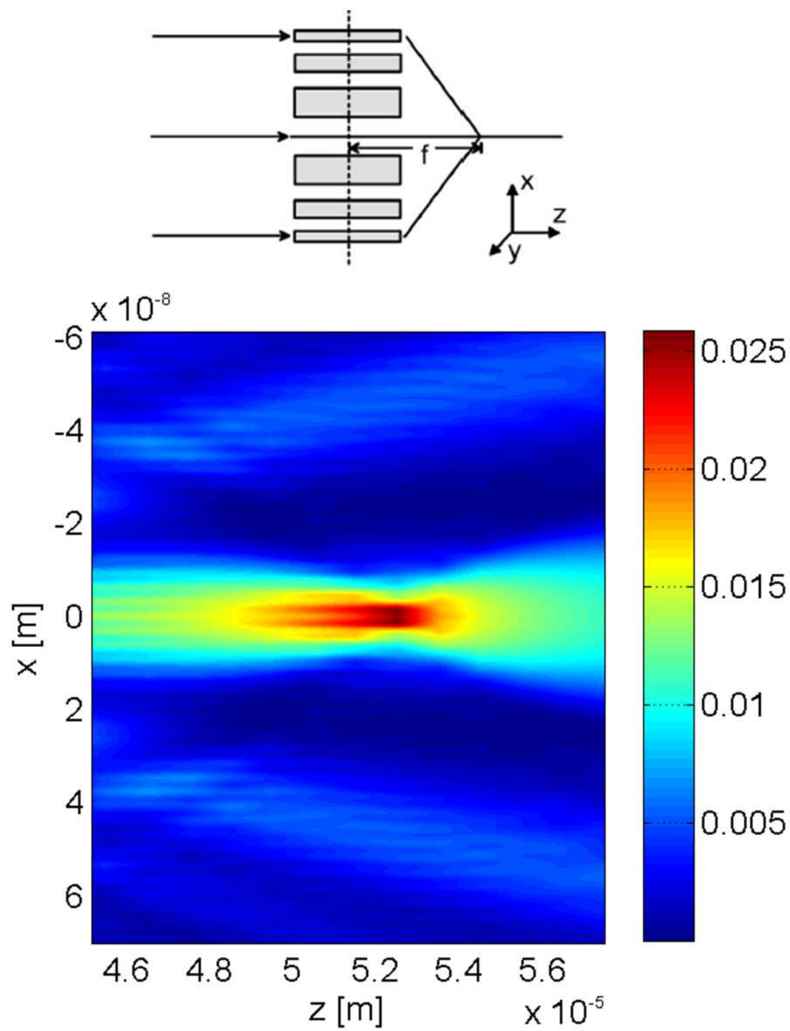
J. Gauden et.al., Optical Letters (2012) , in press

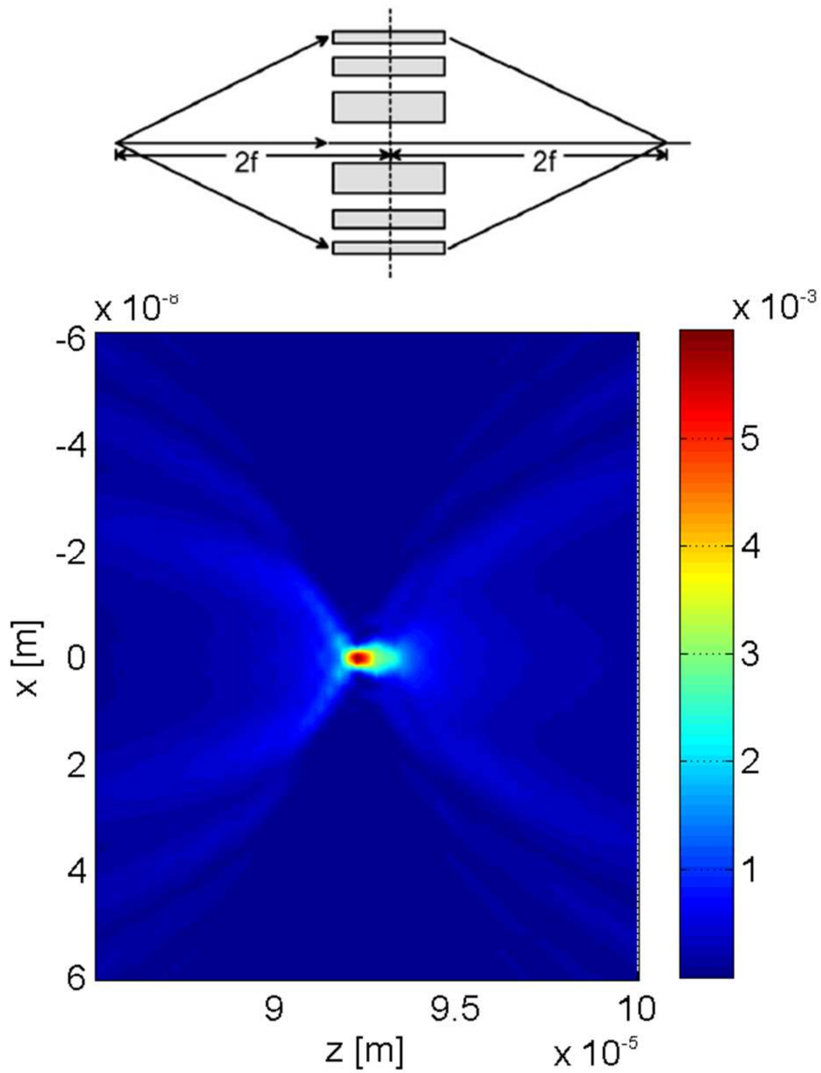
Multilayer Laue lenses (MLL)

$$\frac{\partial \psi(\mathbf{r}_\perp, z)}{\partial z} = \frac{i}{2}[\nabla_\perp \psi(\mathbf{r}_\perp, z) + \boxed{\delta\varepsilon(\mathbf{r}_\perp, z)}\psi(\mathbf{r}_\perp, z)]$$



Thick Fresnel Zone Plate, outer zone 1.5 nm thick





Benchmarking w/r to eigenfunctions expansion method

$$\Psi(x,z) = e^{\mathrm{i}kEz}\psi(x), \tag{6}$$

we obtain the time-independent Schrödinger equation

$$H\psi = E\psi. \tag{7}$$

Let $\{\psi_n\}$ be the eigenfunctions of H and $\{E_n\}$ the corresponding eigenvalues

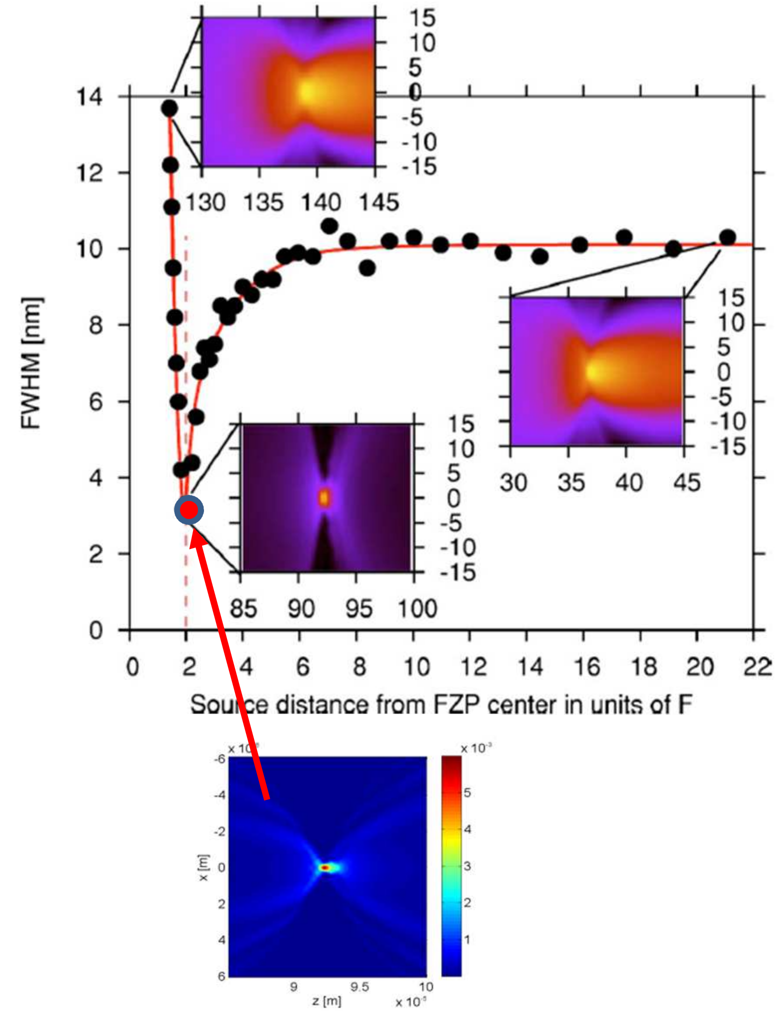
$$H\psi_n = E_n\psi_n. \tag{8}$$

The incoming wavefield $\langle x|\Psi_{\mathrm{in}}\rangle \equiv \Psi_{\mathrm{n}}(x, z=-h/2)$ is decomposed in eigenfunctions

$$|\Psi_{\mathrm{in}}\rangle = \sum_n \langle\psi_n|\Psi_{\mathrm{in}}\rangle|\psi_n\rangle. \tag{9}$$

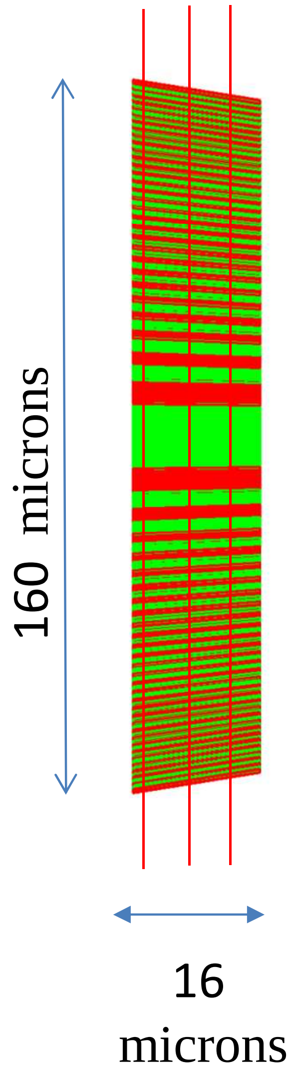
After propagation within the zone plate over its thickness h the wave function has evolved to the exit wavefield $\langle x|\Psi_{\mathrm{ex}}\rangle \equiv \Psi_{\mathrm{ex}}(x, z=h/2)$, with

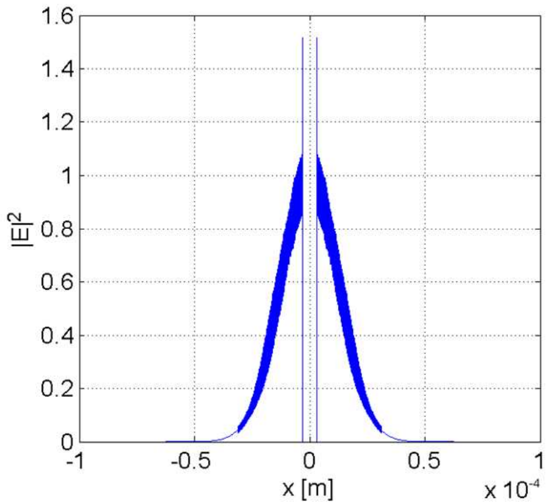
$$|\Psi_{\mathrm{ex}}\rangle = \sum_n \langle\psi_n|\Psi_{\mathrm{in}}\rangle e^{\mathrm{i}kE_nh}|\psi_n\rangle. \tag{10}$$

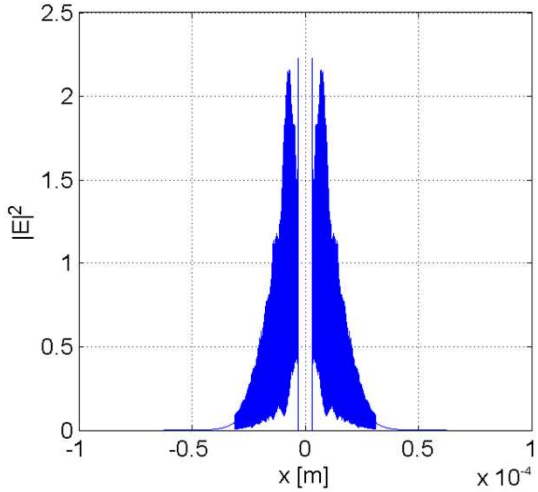


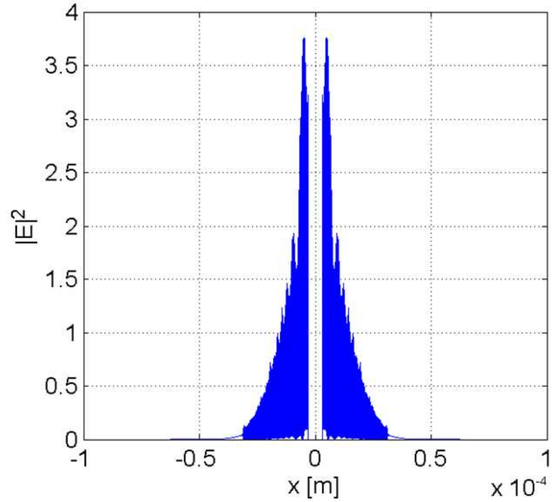
PFEIFFER *et al.* , Phys. Rev. B **73, 245331 2006**

MLL wedged lens, outer layer 1 nm thick, photon energy 19.5 keV





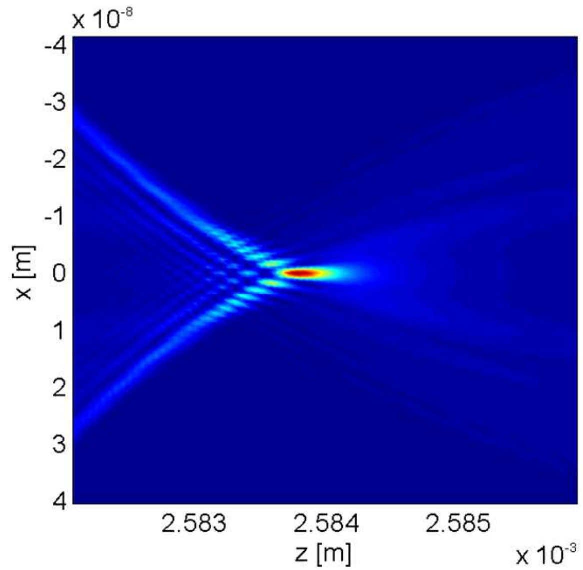




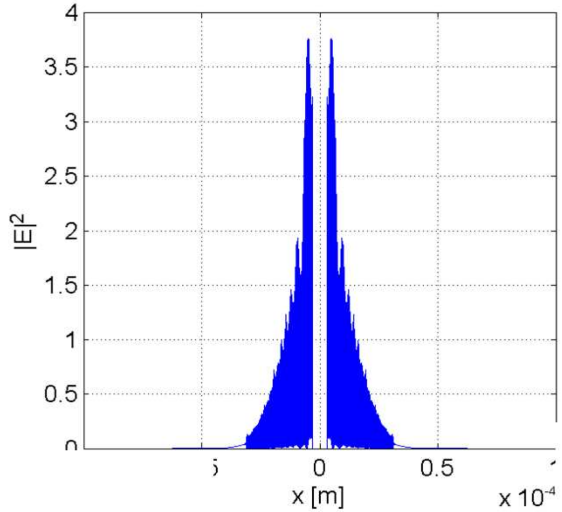
$$x_j^2 = \left(j\lambda f + \frac{j^2\lambda^2}{4}\right)a(z)^2, \quad a(z) = 1 - \frac{z}{2f}.$$

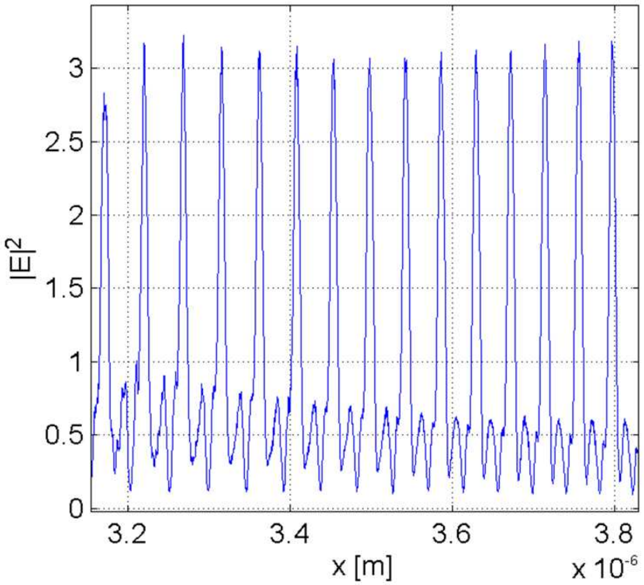
Focal length 2.6 mm

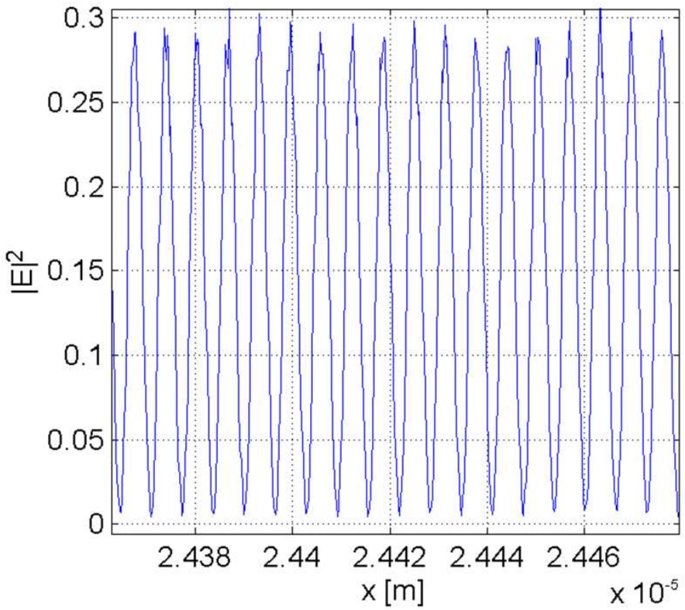
Focus size 1.5 nm WHHM



Electric field distribution inside MLL

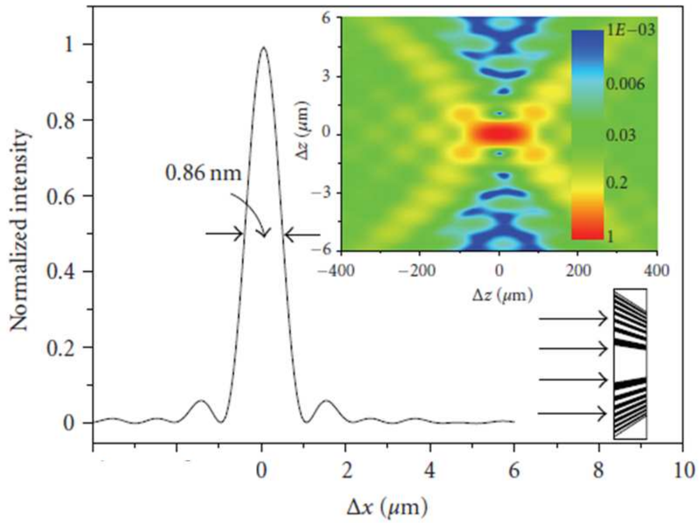






Comparison with dynamical diffraction theory

a modeling method that is analogous to Takagi-Taupin equations in crystallography by realizing the similarities of X-ray diffraction between an MLL and a single crystal [18].



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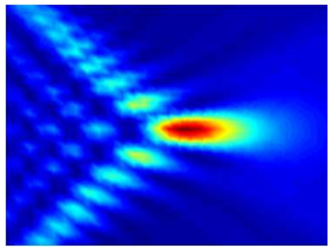


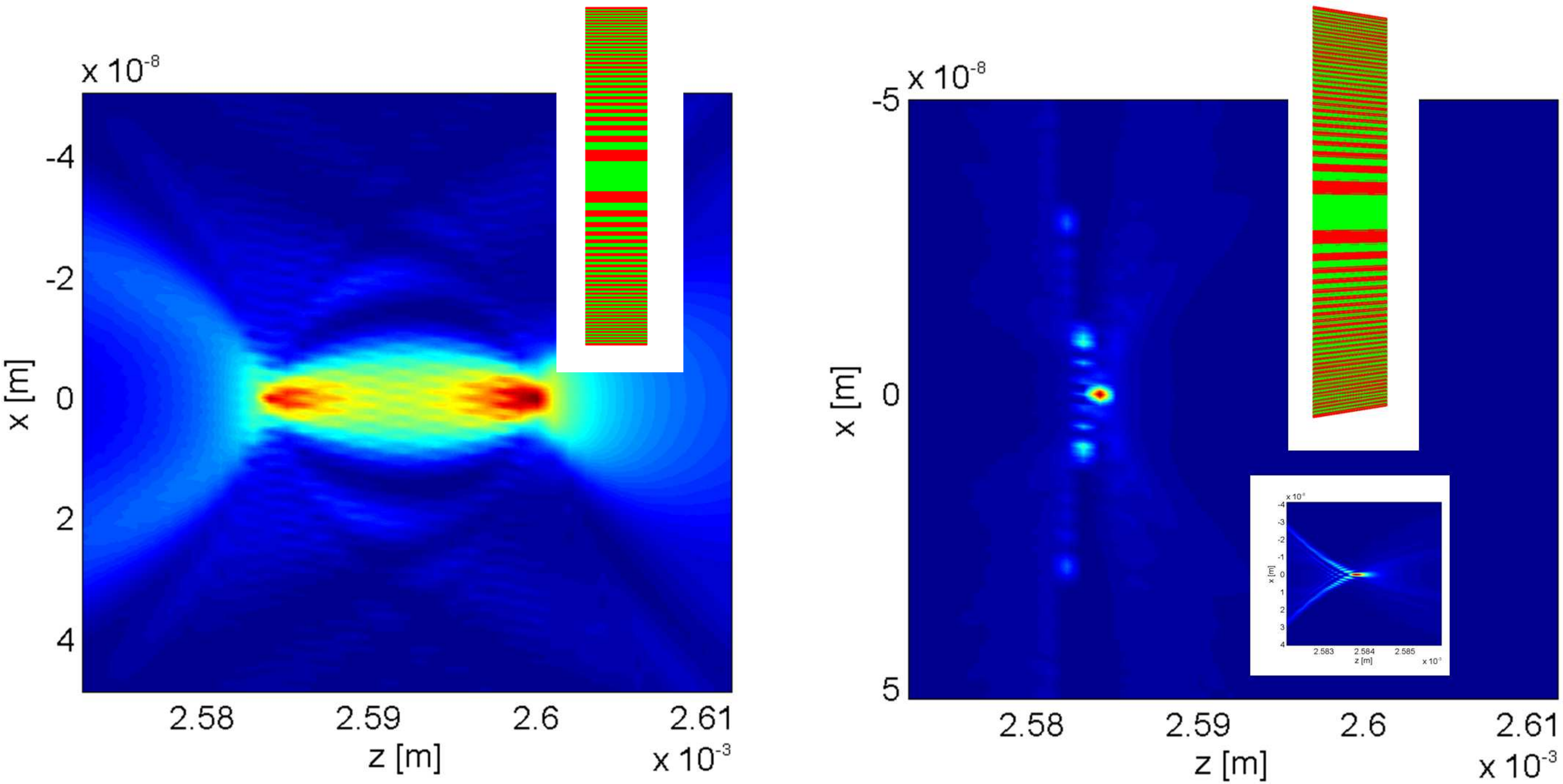
BPM simulation

Review Article

Multilayer Laue Lens: A Path Toward One Nanometer X-Ray Focusing

Hindawi Publishing Corporation
X-Ray Optics and Instrumentation
Volume 2010, Article ID 401854, 10 pages
doi:10.1155/2010/401854

Focusing of thick FZP and wedged MLL, outer zone is 1 nm thick



Outlook

- I hope that I convinced you that:
- BPM can be applied successfully in the wide range or problems
- It is simple and computationally efficient
- It is especially convenient for simulating the influence of imperfections as they can be naturally included in the model