

Simulation of XFEL pulse propagation through double crystal Laue monochromator



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Motivation

European
XFEL



Web cams, September 2010

Motivation



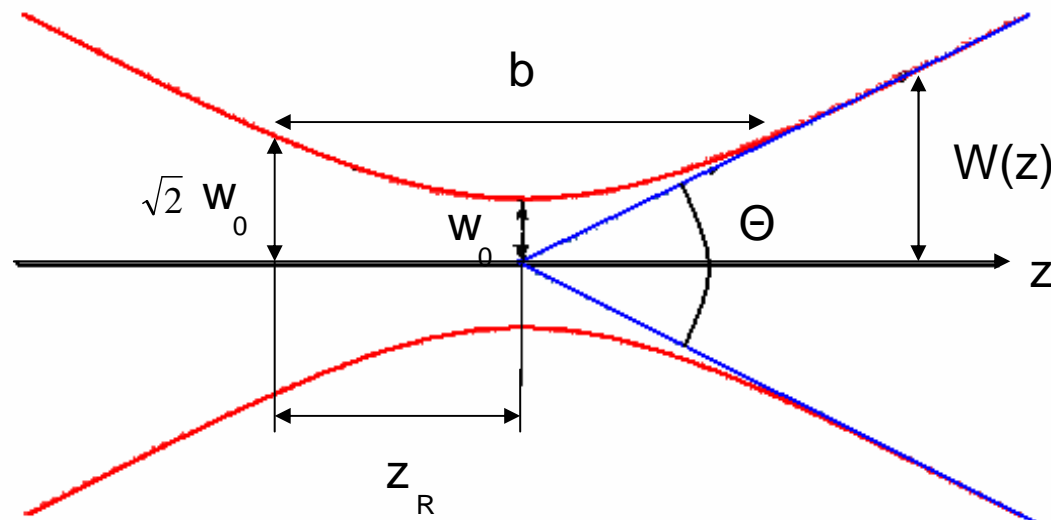
Crystal monochromator for synchrotron radiation:

- For most cases Bragg geometry
- Si perfect crystals
- Band pass ($\Delta E/E$) defined by beam divergence
- Non- or partially coherent source

Crystal monochromator for European XFEL:

- Laue geometry
 - Diamond crystals
 - Angular divergence $\sim 1 \mu\text{rad} \ll \Delta\theta_{\text{crystal}}$
 - Almost fully transverse coherent source
- } to survive in extremely high peak heat loads
- } approximated by Gaussian beam

Gaussian beam



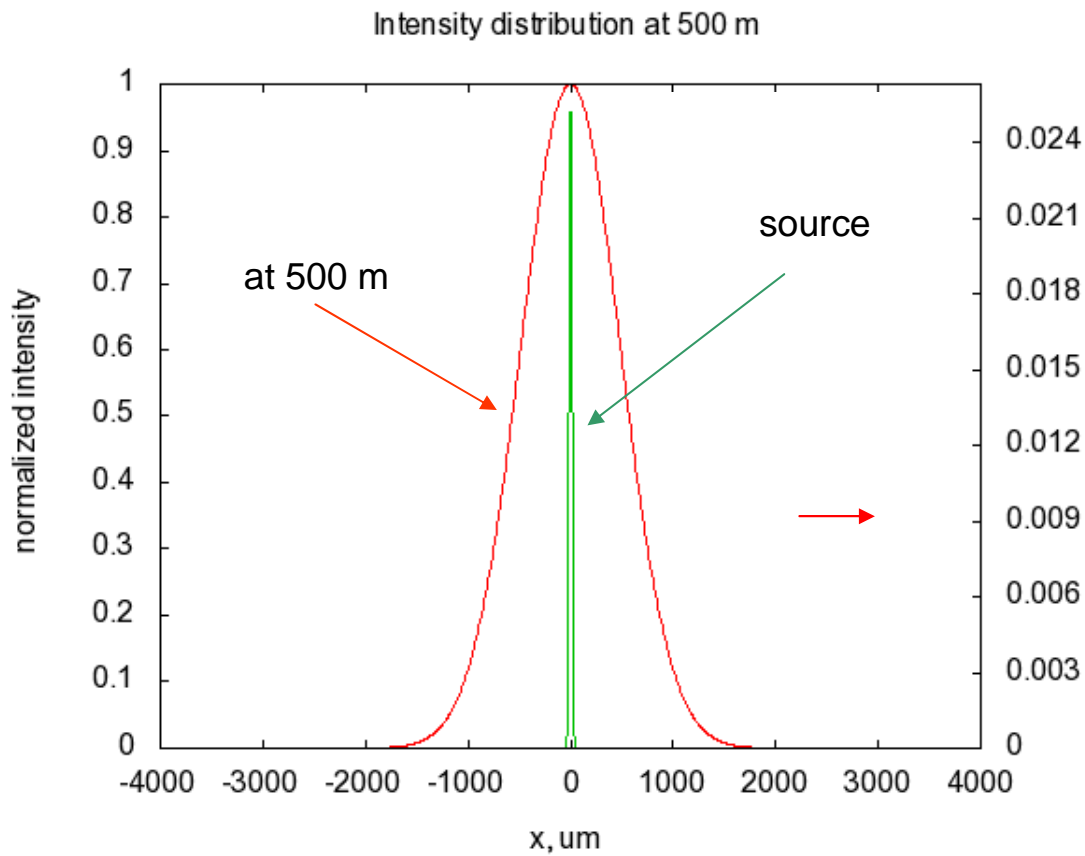
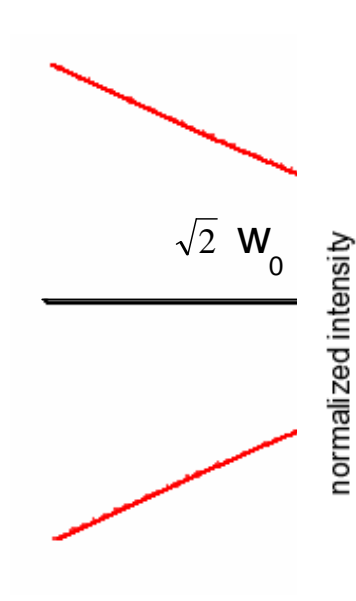
$$\theta \cong \frac{\lambda}{\pi w_0}$$

θ - angular divergence

λ - wavelength

w_0 - beam waist width

Gaussian beam



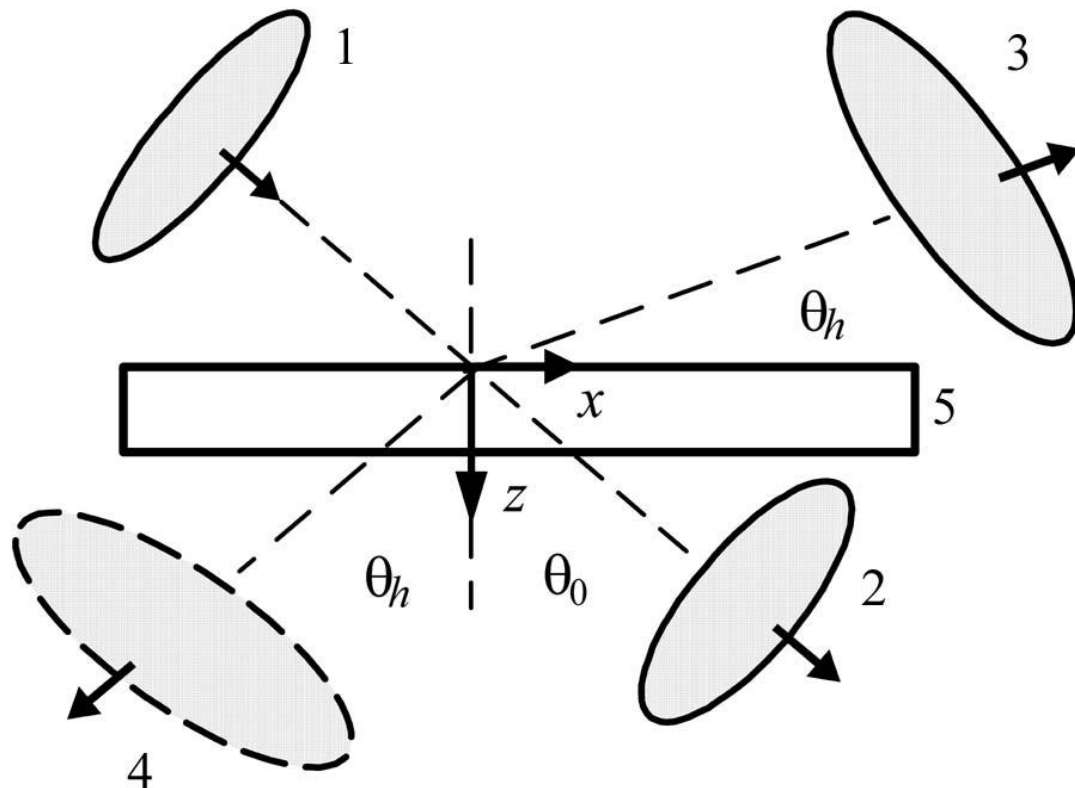
$$\frac{\lambda}{w_0}$$

divergence

1/2

size

Dynamical diffraction theory



$$R(y) = \left| \frac{\chi_h}{\chi_{\bar{h}}} \right| \frac{\sin^2(A\sqrt{1+y^2})}{1+y^2},$$

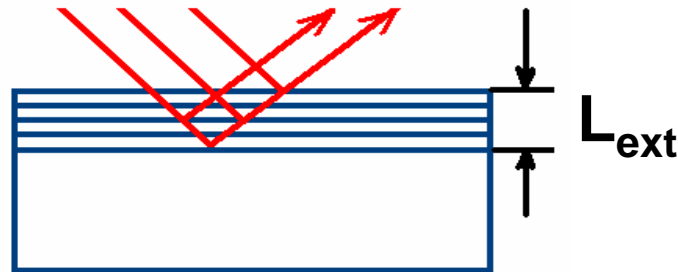
$$A = \pi \frac{t}{L_{ext}},$$

V.A. Bushuev, JSR, 2008, p.495-505

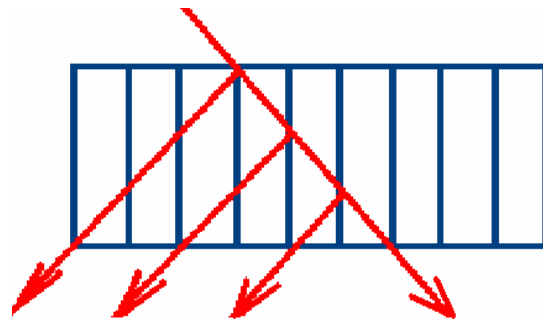
Dynamical diffraction theory: extinction length



Bragg case
thick crystal
Extinction



Laue case
non-absorbing crystal
Pendellösung



$$L_{ext} = \lambda \frac{\sqrt{|\gamma_0 \gamma_h|}}{\pi |\operatorname{Re}(\chi_h)|},$$

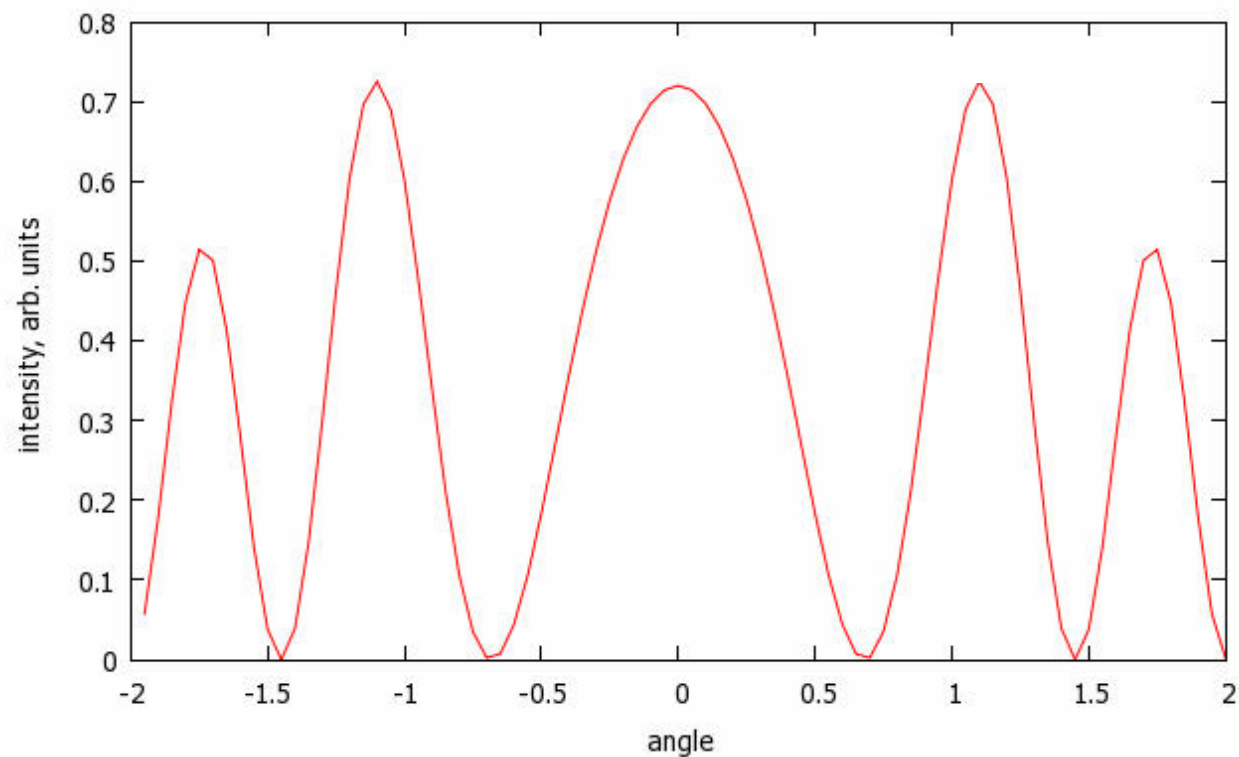
$$\gamma_h = \cos(\Theta_h),$$

$$\gamma_0 = \cos(\Theta_0),$$

$$R(y) = \left| \frac{\chi_h}{\chi_h^-} \right| \frac{\sin^2(A\sqrt{1+y^2})}{1+y^2}, \quad A = \pi \frac{t}{L_{ext}},$$

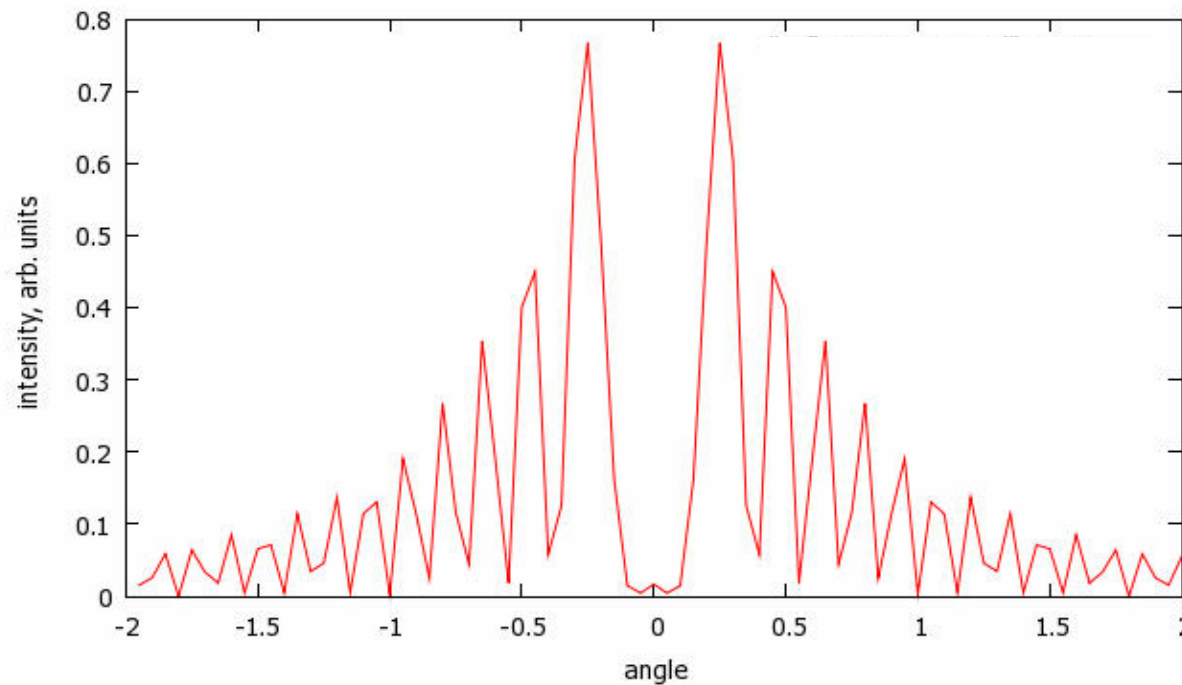
Pendellösung solution

$$t = \frac{\pi}{2} L_{ext} (2n + 1), \quad \text{where } n=0,1,2,\dots \text{ is an integer}$$



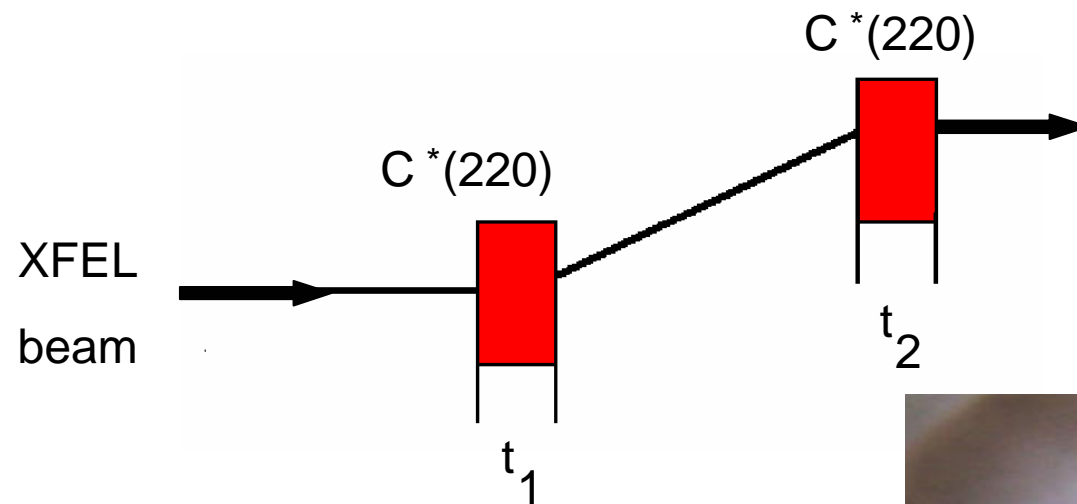
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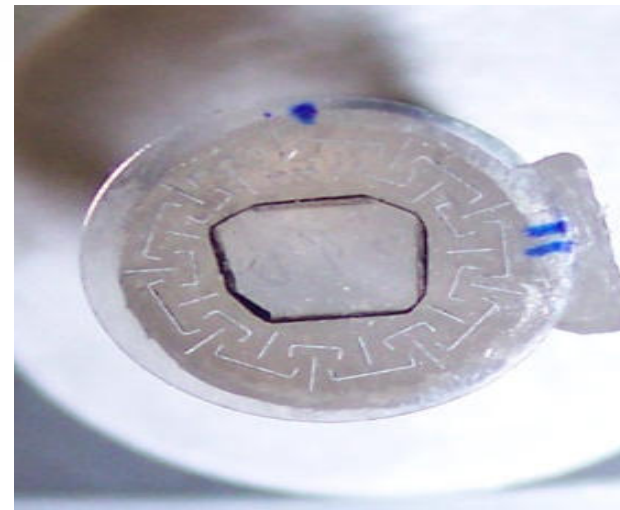


$$L_{ext} = \lambda \frac{\sqrt{|\gamma_0 \gamma_h|}}{\pi |\operatorname{Re}(\chi_h)|},$$

Double crystal monochromator (DCM)



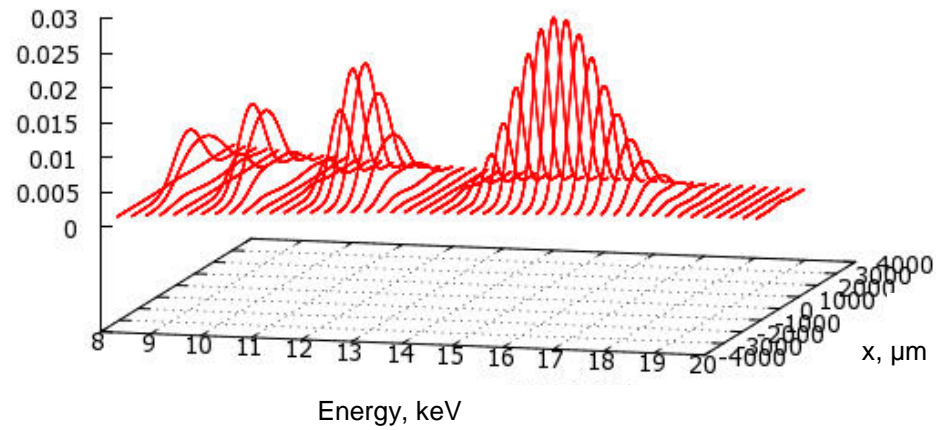
Diamond (100)



Results



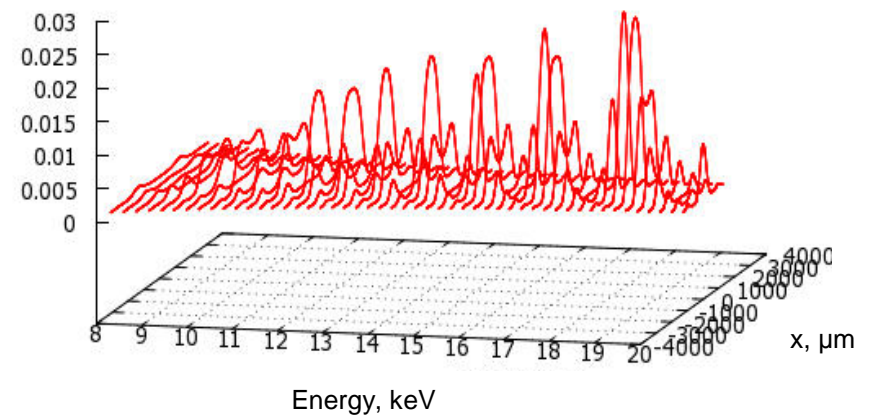
Intensity, arb. units



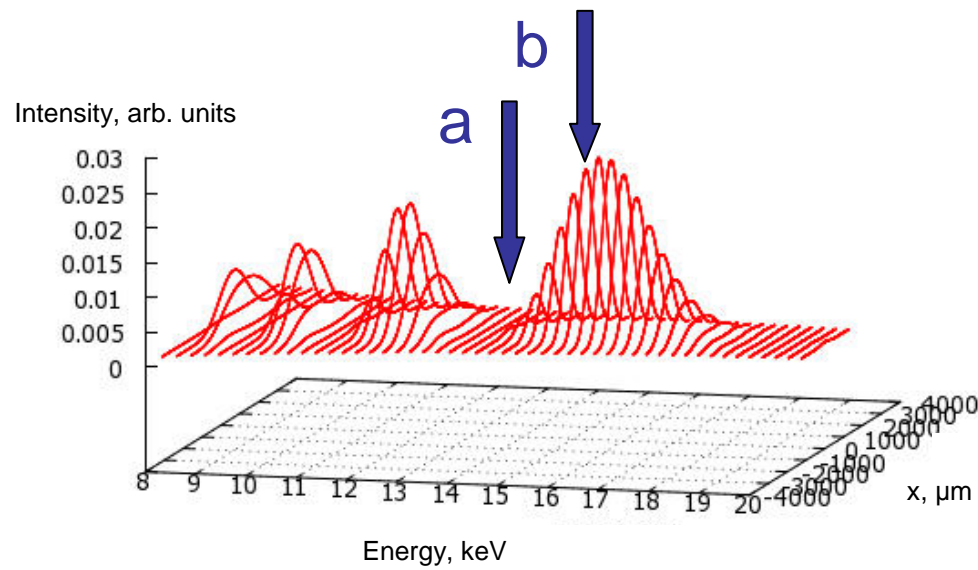
Crystals thicknesses 98 μm

Crystals thicknesses 400 μm

Intensity, arb. units

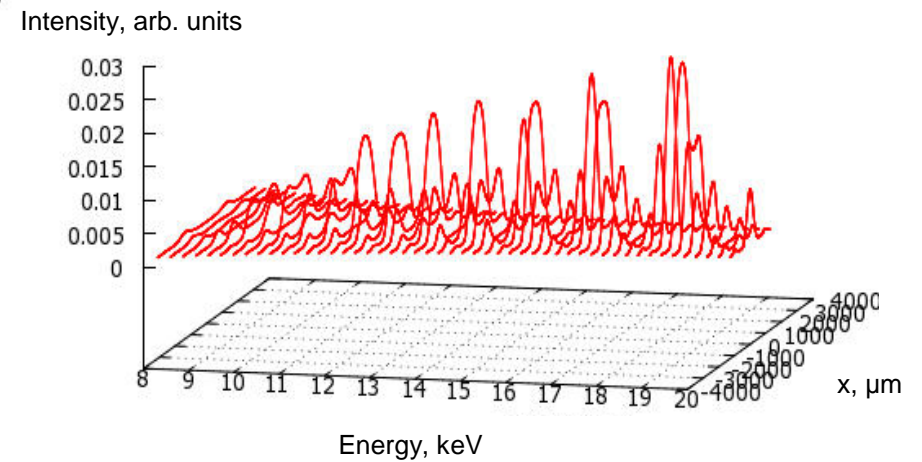


Results



Crystals thicknesses 98 μm

Crystals thicknesses 400 μm

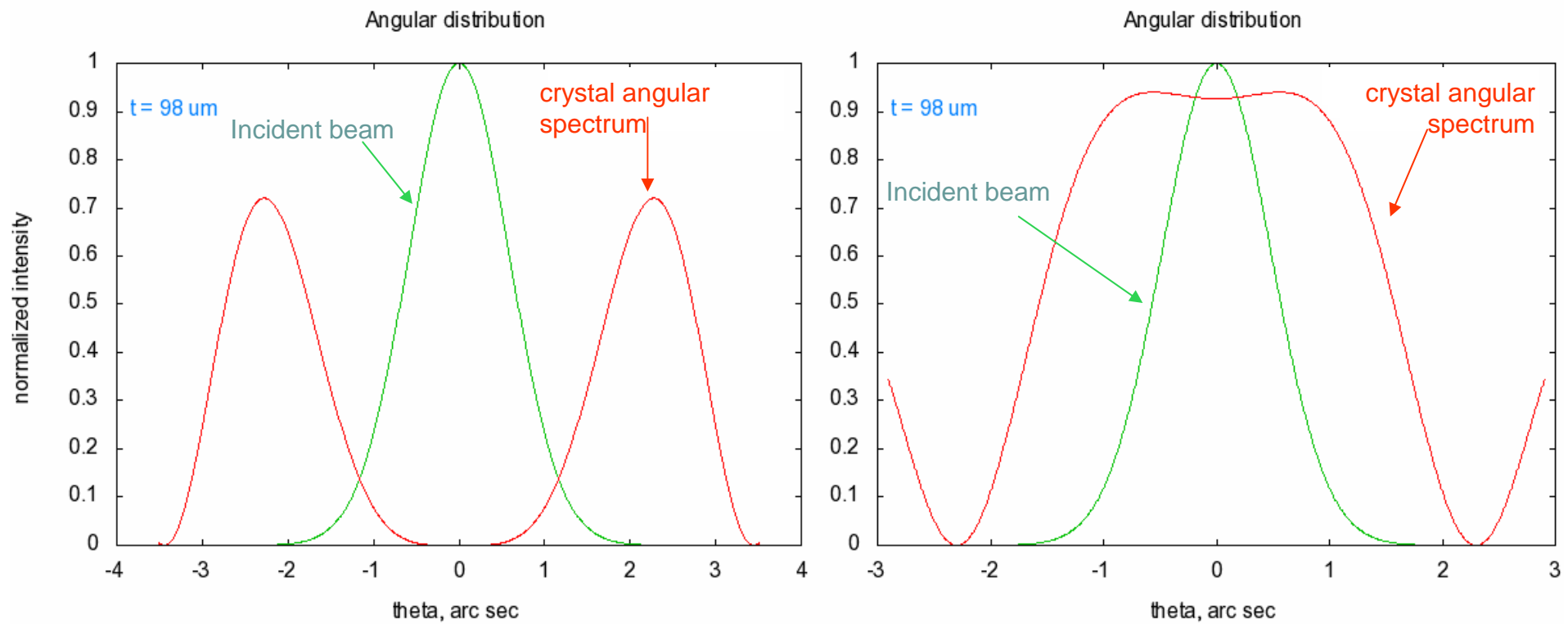


Reflection curves and beam position



a, E=13 keV

b, E=16 keV

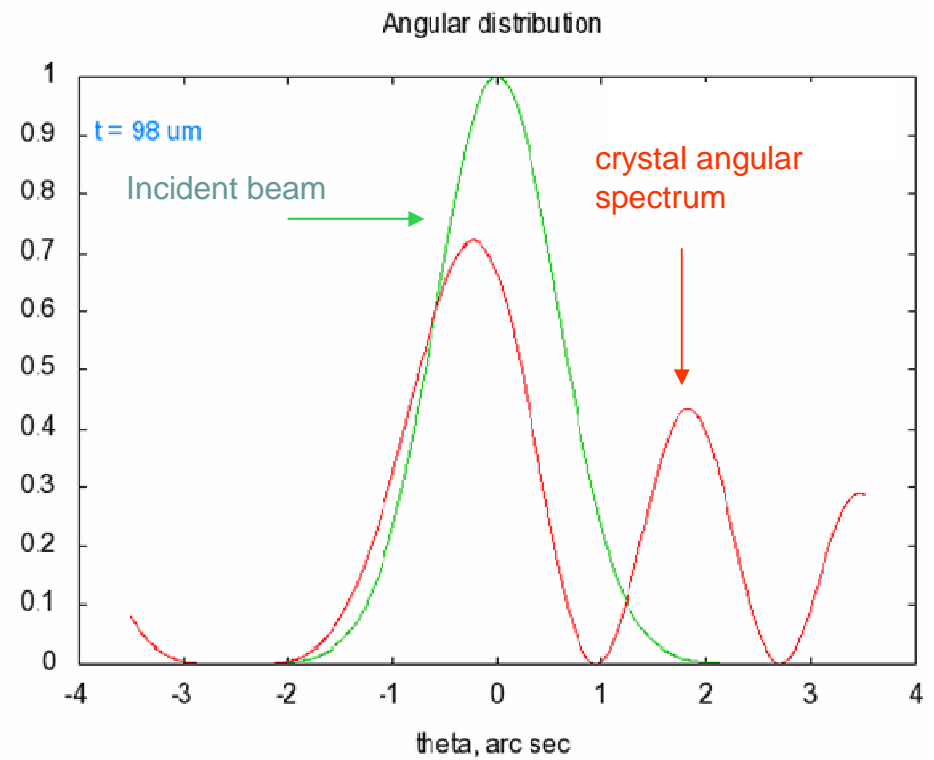
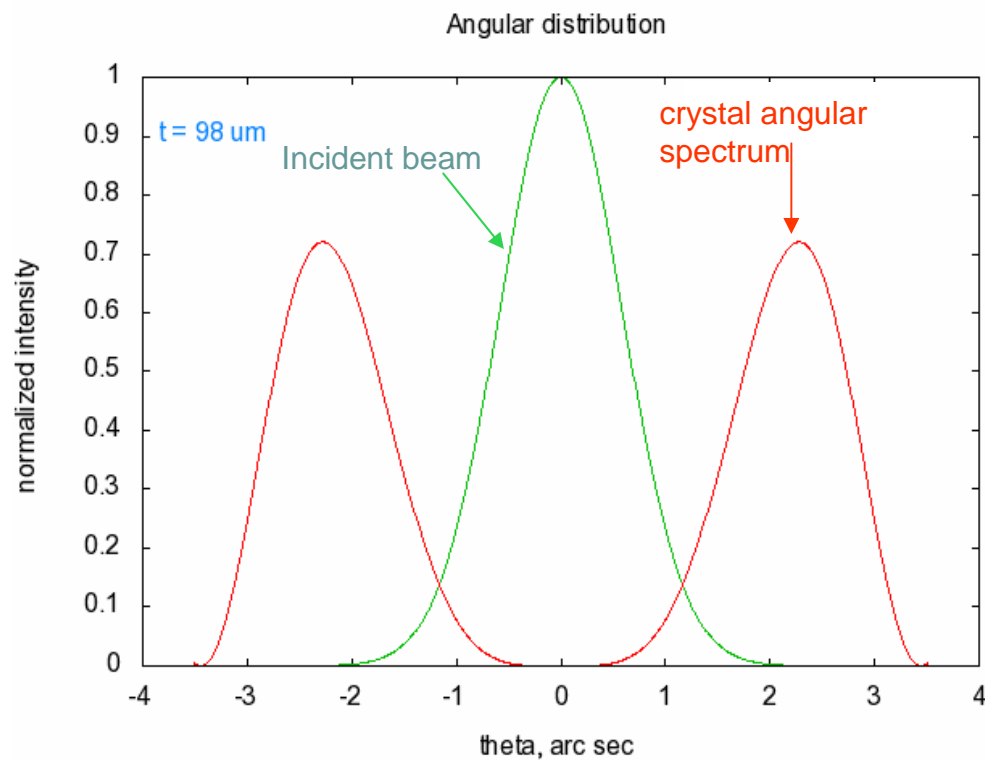


Reflection curves and beam position



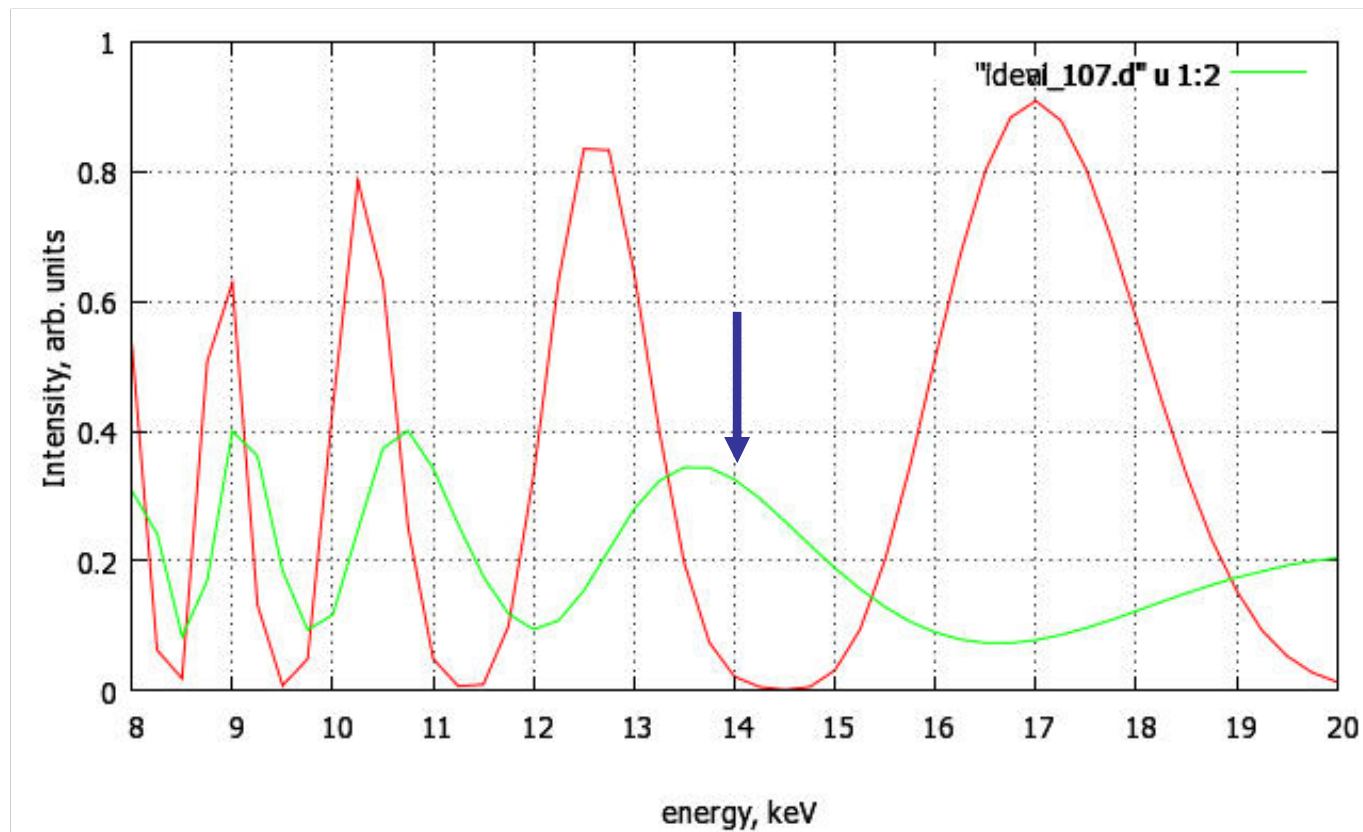
a, $E=13$ keV

a, $\Delta\theta = 2.5$ arc. sec.



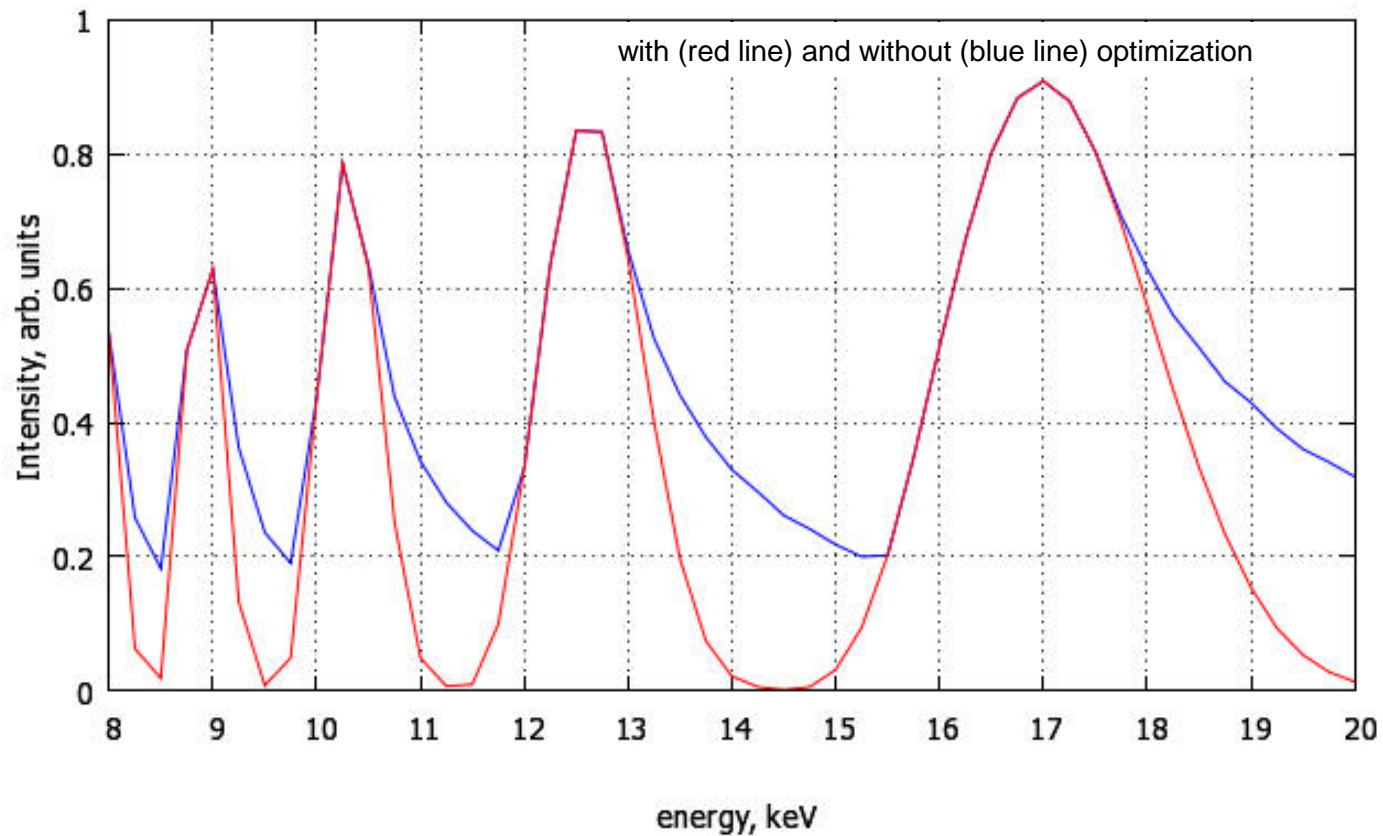
Integral intensity

crystal thickness 107 μm , angle deviation (green line) 2.5 arc. sec.



Optimized integral intensity

crystal thickness 107 μm , angle deviation for red line was optimized for each step



Conclusions and outlook



- Slight asymmetry (~ 1 deg)
- Small deviations from exact Bragg angle ($< 1 \mu\text{rad}$)
- Crystals thickness variation within few microns

are not
critical

- Small thickness crystals (about $100 \mu\text{m}$) seems to be more suitable.
- Crystal thickness can't be optimized for entire energy range (8-20 keV).
- Environment for Laue DCM optimization was developed and can be used for further simulations.

Next step:

- Simulations, taking into account time dependence. For instance, two short pulses separate in time.

Acknowledgments



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- V. Bushuev (Moscow State University)

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Thank You for attention