

Diffraction of ultrashort pulses of hard X-ray FEL radiation by single crystals.

**Bragg and Laue cases, effects
of time coherence.**

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The brief plan:

1. The basic parameters of XFEL pulses
2. Pulse propagation in free space
3. Features of diffraction of femtosecond X-ray pulses in Bragg and Laue cases
4. Influence of statistical properties of XFEL pulses on diffraction reflection and transmission

Рентгеновский лазер на свободных электронах (РЛСЭ)

X-ray Free Electron Laser (XFEL)

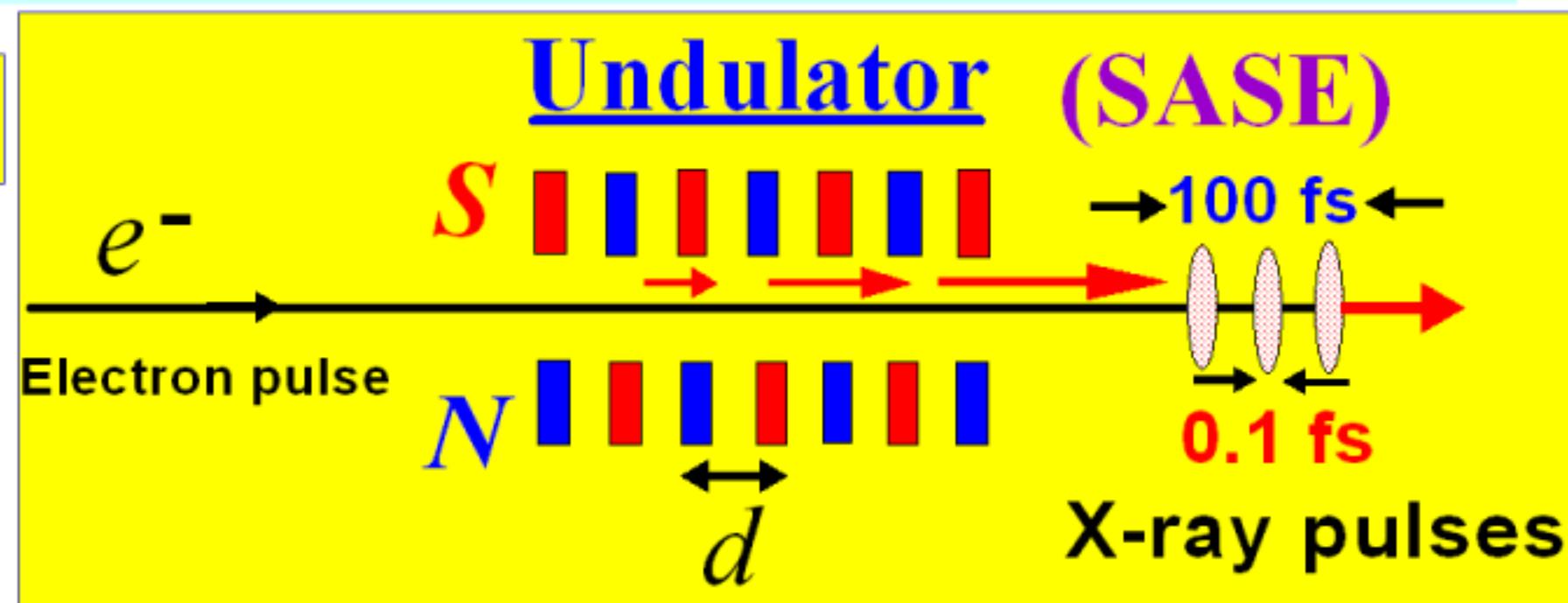
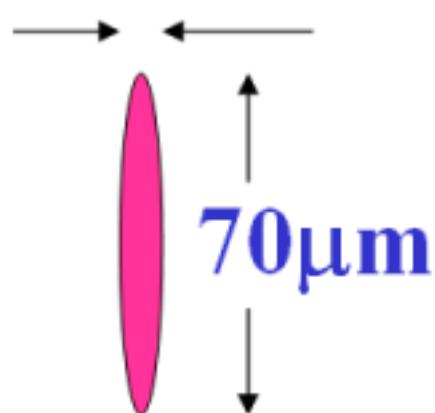
- Projects:
1. European XFEL (Germany, Hamburg)
 2. LCLS (USA, Srenford)
 3. Japanese XFEL (Japan, SPring 8)

$$1 \text{ fs} = 10^{-15} \text{ s}$$

$$\frac{r_0}{c\tau_s} \approx 10^3$$



30 nm

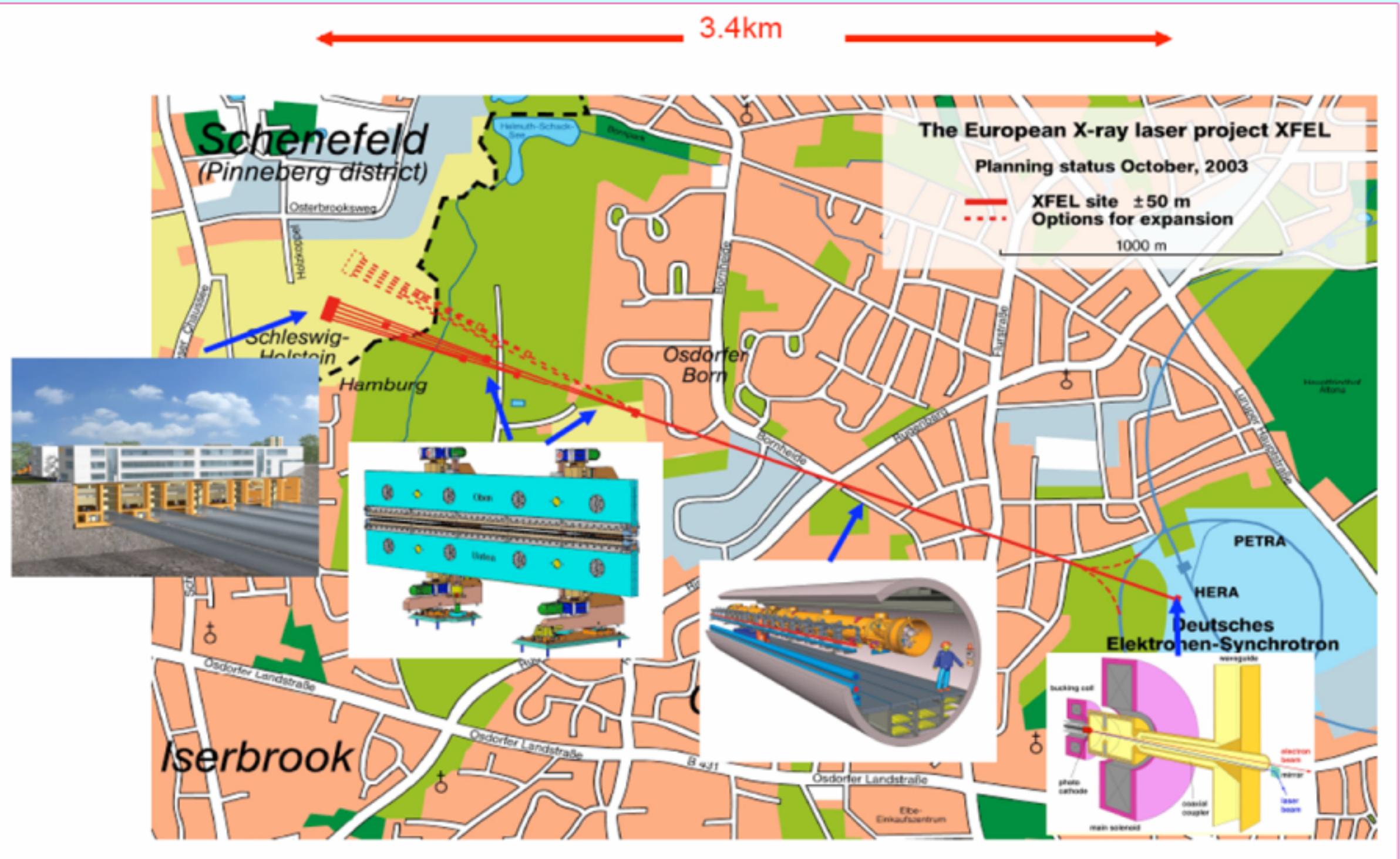


$$\lambda \approx d(1+K^2)/2\gamma^2$$

$$\Delta\lambda/\lambda \approx 1/2N$$

where $\gamma = E_e/mc^2$, $K = eHd/(2\pi mc^2)$

If $d = 35.6 \text{ mm}$, $E_e = 17.5 \text{ GeV}$, $\lambda \approx 0.1 \text{ nm}$



The scheme and arrangement of XFEL elements
SASE - Self Amplification Spontaneous Emission
("самоусиливающаяся спонтанная эмиссия").

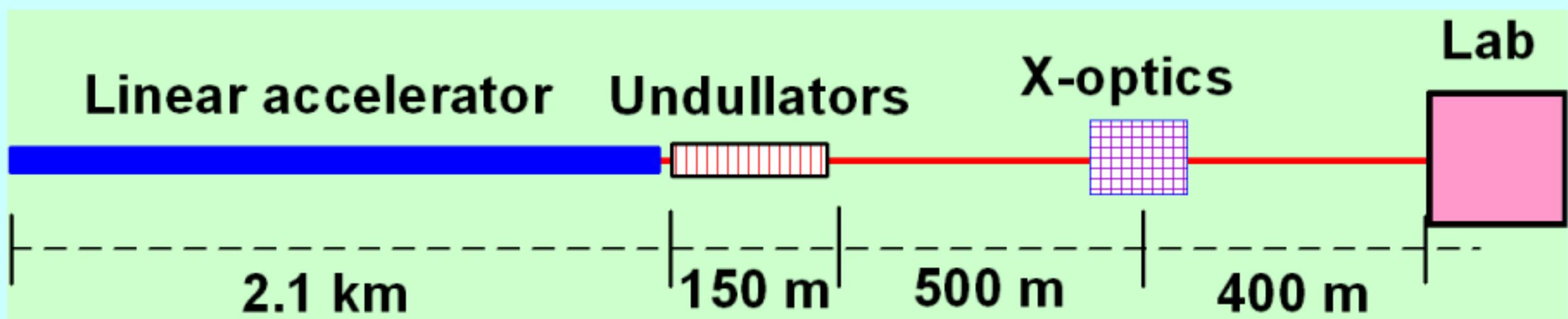
SASE-1 XFEL parameters:

$E \approx 17 \text{ GeV}$, $\Delta\tau \approx 100 \text{ fs}$, $\tau_0 \sim 0.1\text{-}0.2 \text{ fs}$,
 $\delta\tau \sim 0.3\text{-}0.5 \text{ fs}$; $r_0 \sim 50 \mu\text{m}$, $\Delta\theta \approx 1 \mu\text{rad} =$
 $= 0.2 \text{ arc.sec}$, $P_{\max} \approx 10 \text{ GW}$, $P \sim 40 \text{ W}$.

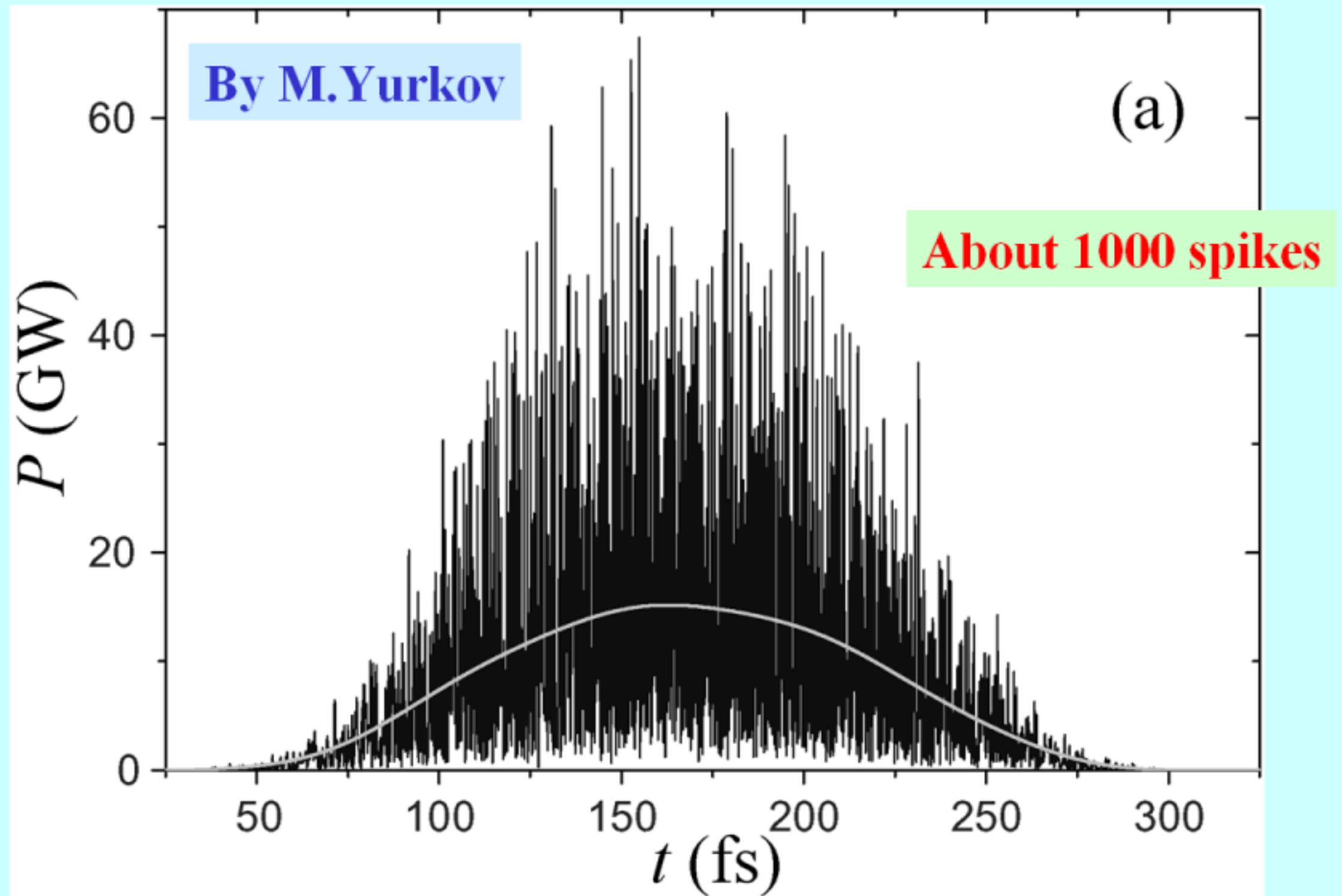
Photons per pulse - 10^{12}

$$\frac{S_{\text{XFEL}}}{S_{\text{SR}}} = 10^9$$

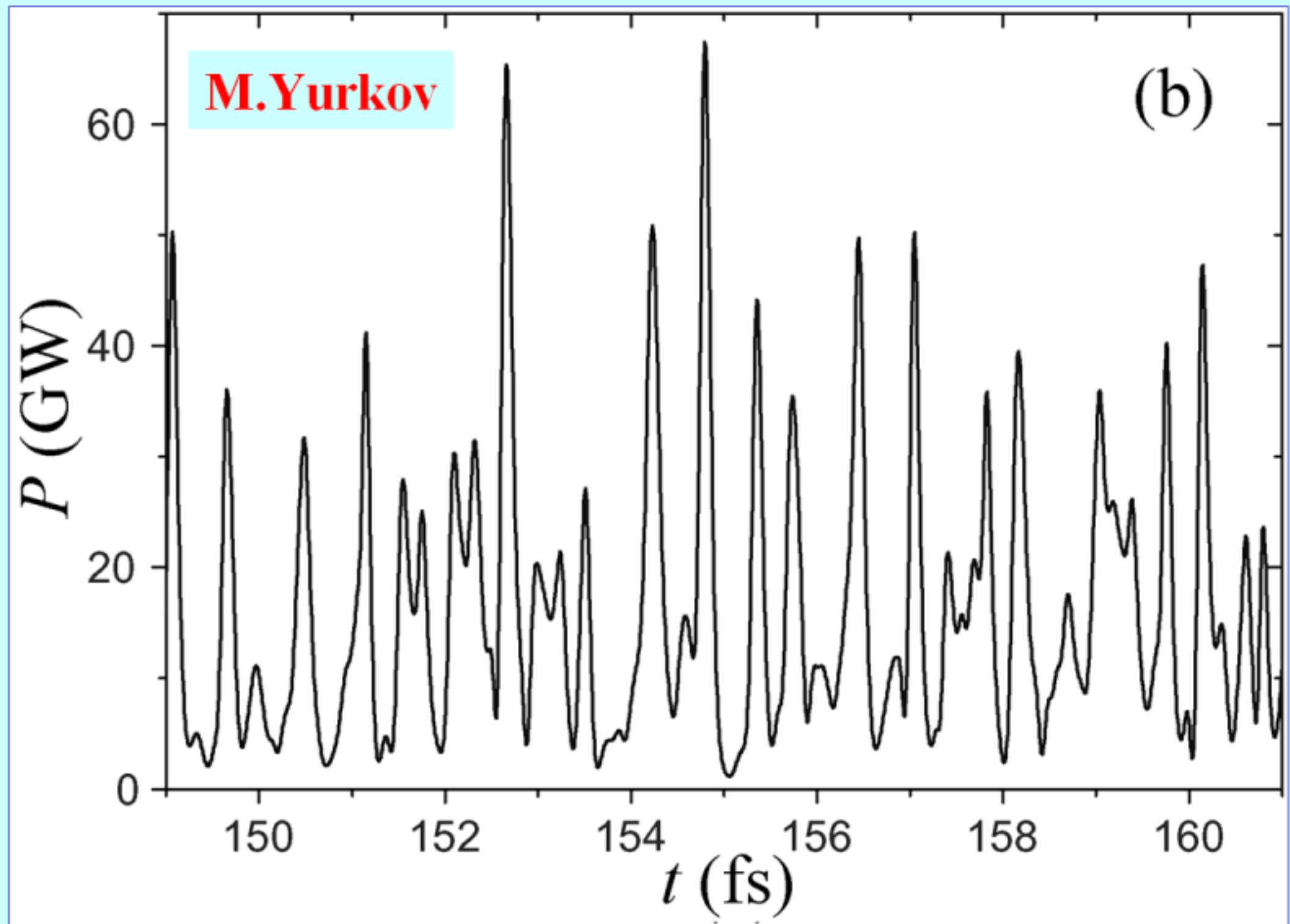
European XFEL distances:



Time structure of a single XFEL pulse



Time structure of a single XFEL pulse fragment



Spike - острый выступ, шип, гвоздь, костьль

The field of XFEL pulse

$$E(\mathbf{r}, z, t) = A(\mathbf{r}, z, t) \exp(ik_0 z - i\omega_0 t)$$

$$\Gamma_{tot}(\mathbf{r}, \mathbf{p}; t, \tau) = \langle A(\mathbf{r}, z, t) A^*(\mathbf{r} + \mathbf{p}, z, t + \tau) \rangle$$

XFEL pulse is **non-uniform in space** and **non-stationary in time**, since its correlation function depend on \mathbf{r} and t
(Wiener-Khinchin theorem does not “work”)

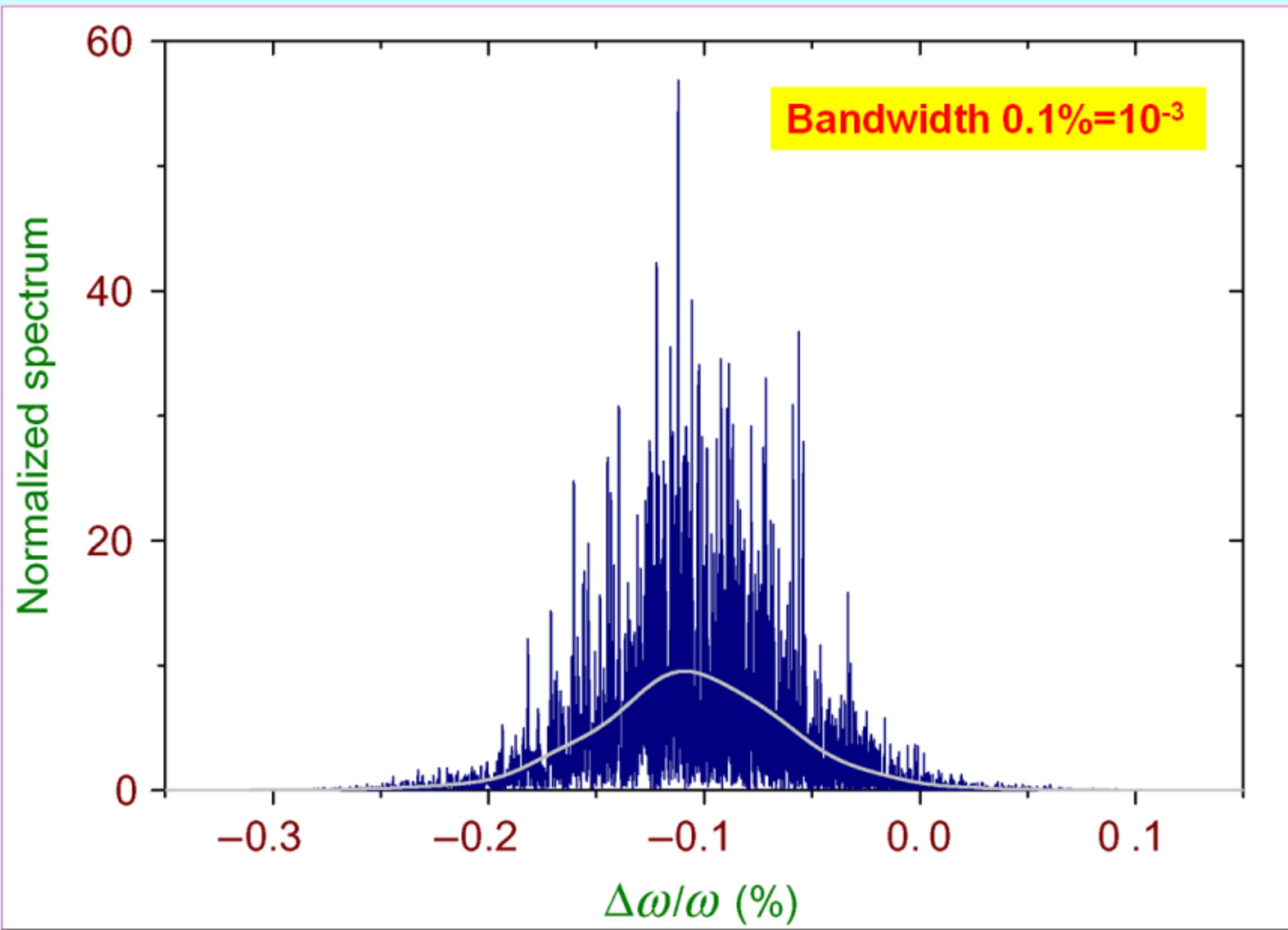
$$A(\mathbf{r}, z, t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} A_s(\mathbf{q}, \Omega) \exp[i\mathbf{qr} - iq^2 z/2k - i\Omega(t - z/c)] d\mathbf{q} d\Omega$$

where $k = (\omega_0 + \Omega)/c$

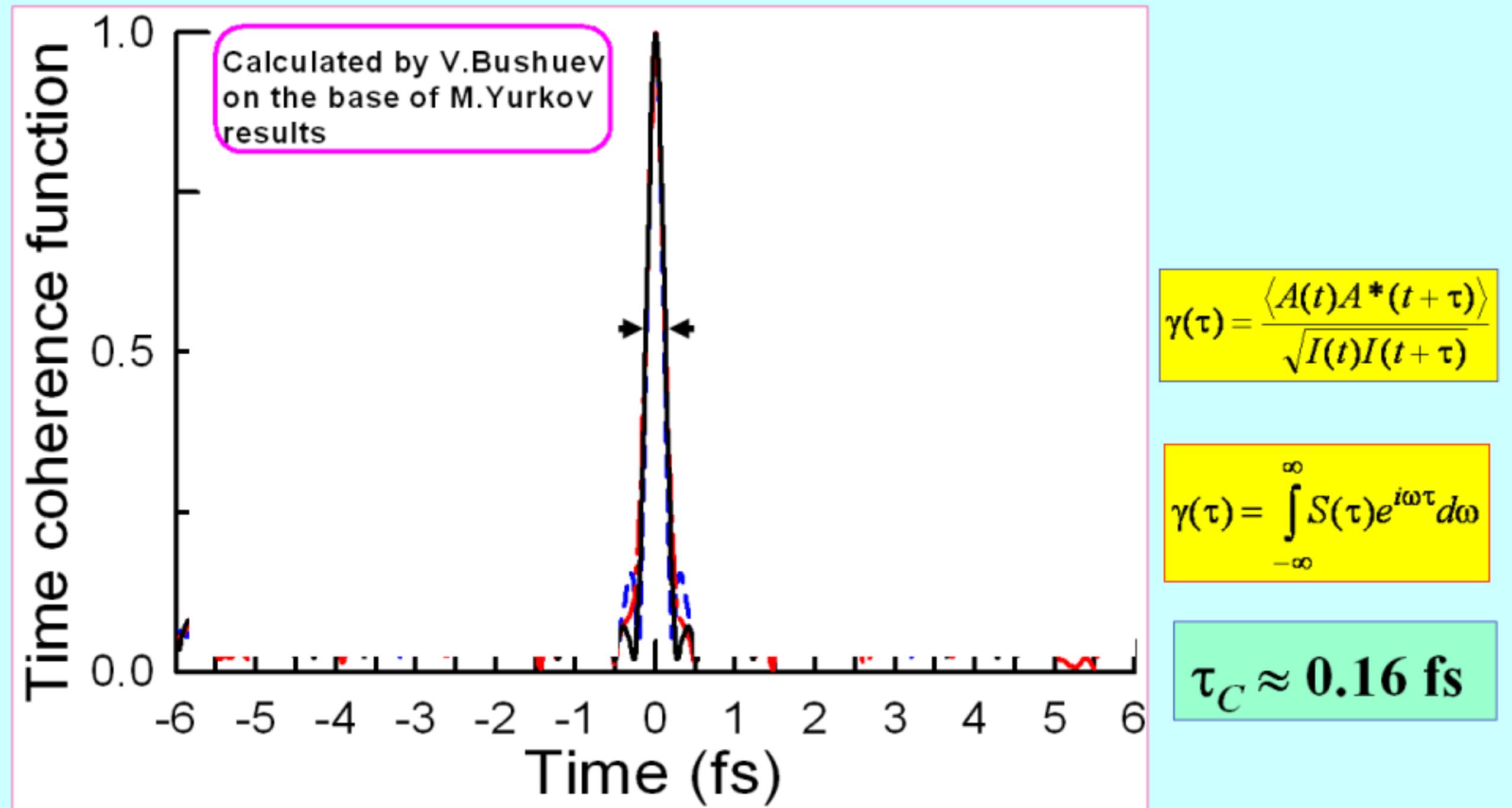
$$k_z = \sqrt{k^2 - q^2} \approx k - q^2/2k$$

The spatial coherence of XFEL at $z=0$ is practically full !!

Spectrum of the XFEL single pulse

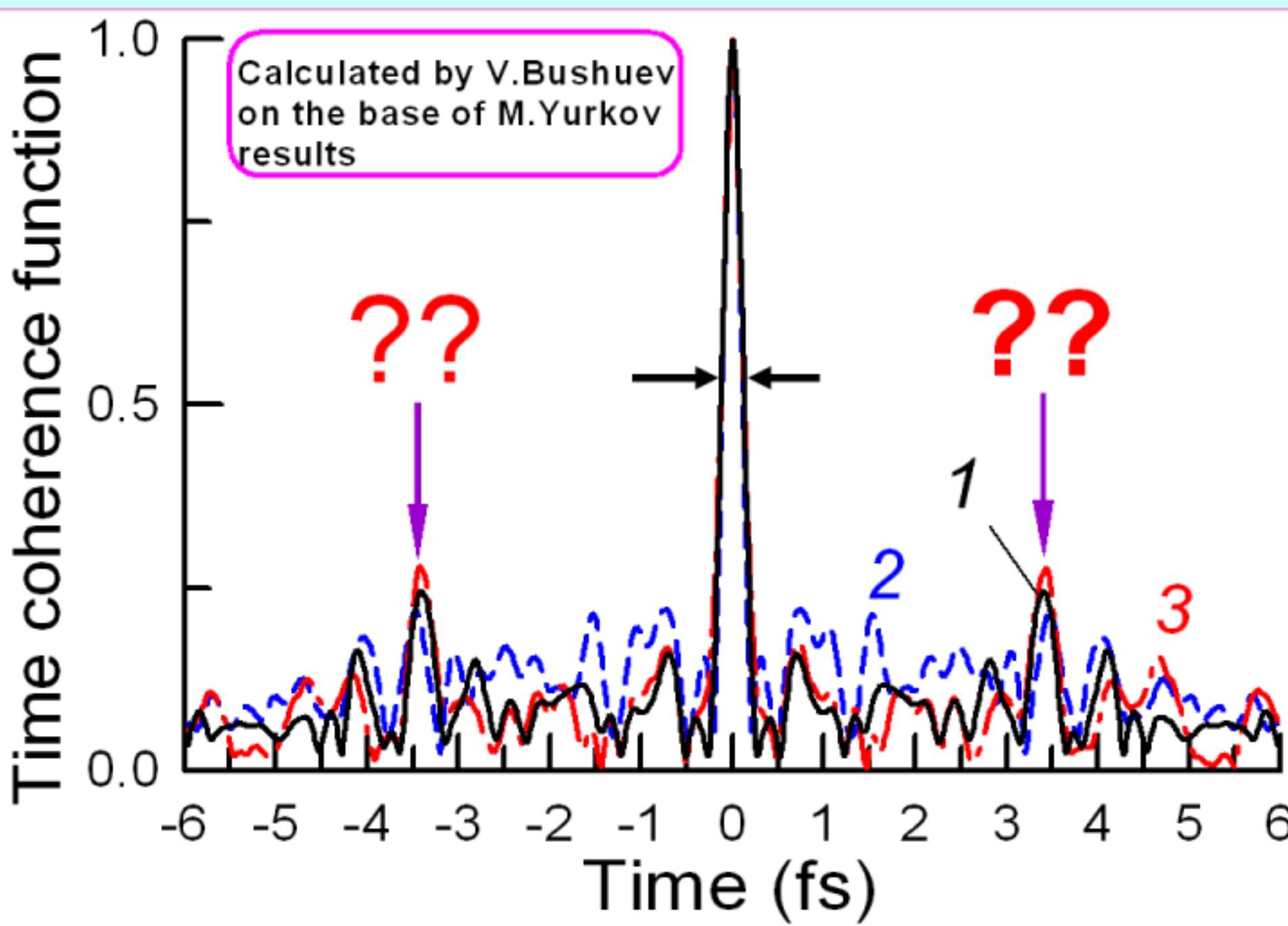


Unusual time coherence function



Unusual time coherence function

$$\tau_C \approx 0.16 \text{ fs}$$



$$\gamma(\tau) = \frac{\langle A(t)A^*(t+\tau) \rangle}{\sqrt{I(t)I(t+\tau)}}$$

$$\gamma(\tau) = \int_{-\infty}^{\infty} S(\omega) e^{i\omega\tau} d\omega$$

If amplitude $A_s(\mathbf{r}, t) = B_s(\mathbf{r})A(t)$, then

$$A(\mathbf{r}, z, t) = B(\mathbf{r}, z)A(t - z/c)$$

$$B(\mathbf{r}, z) = \int_{-\infty}^{\infty} B_s(\mathbf{r}') G(\mathbf{r} - \mathbf{r}', z) d\mathbf{r}'$$

where $G(\xi) = (i\lambda_0 z)^{-1} \exp(i\pi\xi^2/\lambda_0 z)$ - **propagator**

Problem: influence of time coherence
on the spatial coherence ??

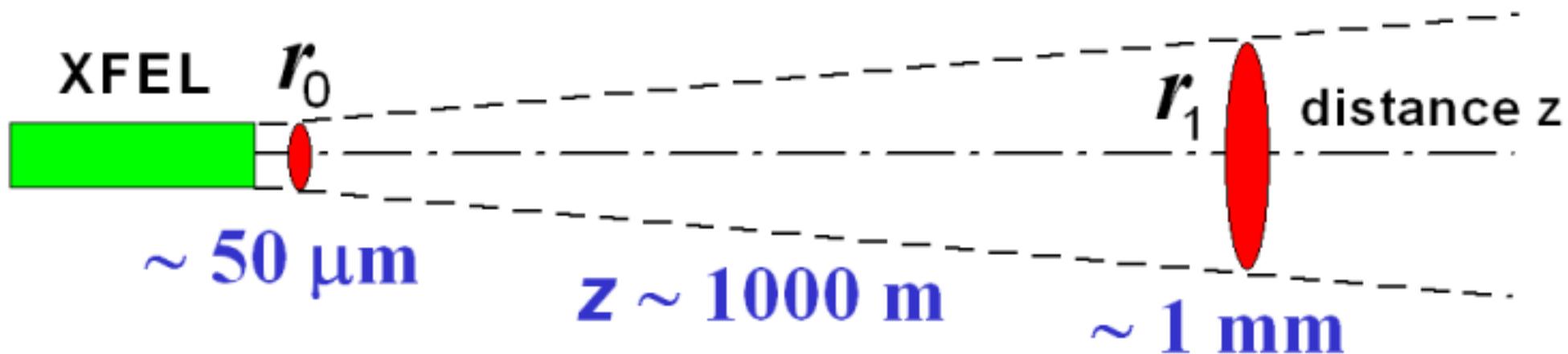
$$z_c \approx 2(\omega_0/\Delta\Omega)k_0 r_0^2$$

If $\Delta\Omega/\omega_0 \sim 10^{-3}$, source size $r_0 \geq 10 \mu\text{m}$, then
critical distance $z_c \geq 10 \text{ km}$

The time structure of the pulse does not vary,
i.e. does not depend on the distance z

$$A(\mathbf{r}, z, t) = B(\mathbf{r}, z) A(t - z/c)$$

$$\Gamma_{tot}(\mathbf{r}, \rho; t, \tau) = \Gamma_\rho(\mathbf{r}, \rho) \Gamma(t, \tau)$$



Gauss pulse size $r_1(z) = r_0 M$,
spatial coherence lenght $\rho_1(z) = \rho_0 M$:

$$M(z) = [(1 + \alpha_0 D)^2 + D^2 + 2DW]^{1/2}$$

where $D = \lambda_0 z / 2\pi r_0^2$, $W = \lambda_0 z / \pi \rho_0^2$

Reduction of the intensity density:

$$\left(\frac{1 \text{ mm}}{50 \mu\text{m}} \right)^2 = 400$$

Film: (x,y) pulse structure at t=150-158 fs

Intensity

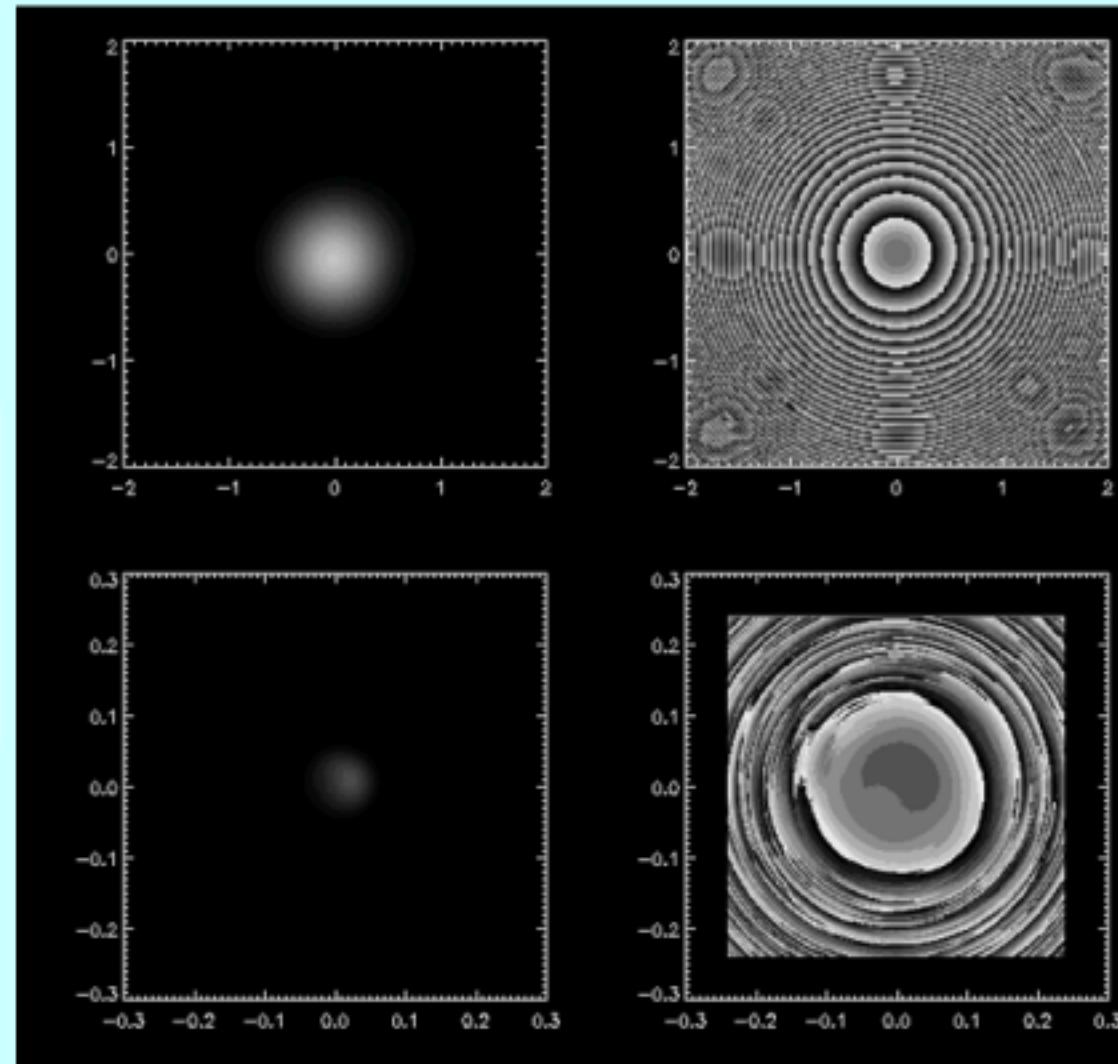
Phase

Distance
 $z = 965$ m

y (mm)

Source
($z = 0$)

x (mm)



Made by L.Samoylova
(base on M.Yurkov 3D-calc.)

Reflected pulse

$$E_R(x, z, t) = \iint R(k_x, \omega) E_0(k_x, \omega) e^{ik_{hx}x - i\sqrt{k^2 - k_{hx}^2}z - i\omega t} dk_x d\omega$$

$$k_{hx} = k_x + h_x, \quad k = \omega/c.$$

$$A_R(x, z, t) = \iint R(q, \Omega) E_0(q, \Omega) e^{i\varphi_S + i\varphi_D} dq d\Omega$$

$$\varphi_S(q, \Omega) = q \times (x - z \operatorname{ctg} \vartheta_R) - \Omega \times \left(t - \frac{z}{c \sin \vartheta_R} \right) \text{ - shift}$$

$$\varphi_D(q, \Omega) = -\frac{1}{2k_0 \gamma_h^3} \left(q - \frac{\Omega \cos \vartheta_R}{c} \right)^2 z$$

- broadening !!

Short pulse diffraction

$$\Delta\theta_{difr} \approx \frac{\lambda}{2r_0} \quad \text{- angular width}$$

$$\Delta\omega_{spectr} \approx \frac{2}{\tau_0} \quad \text{- spectral width}$$

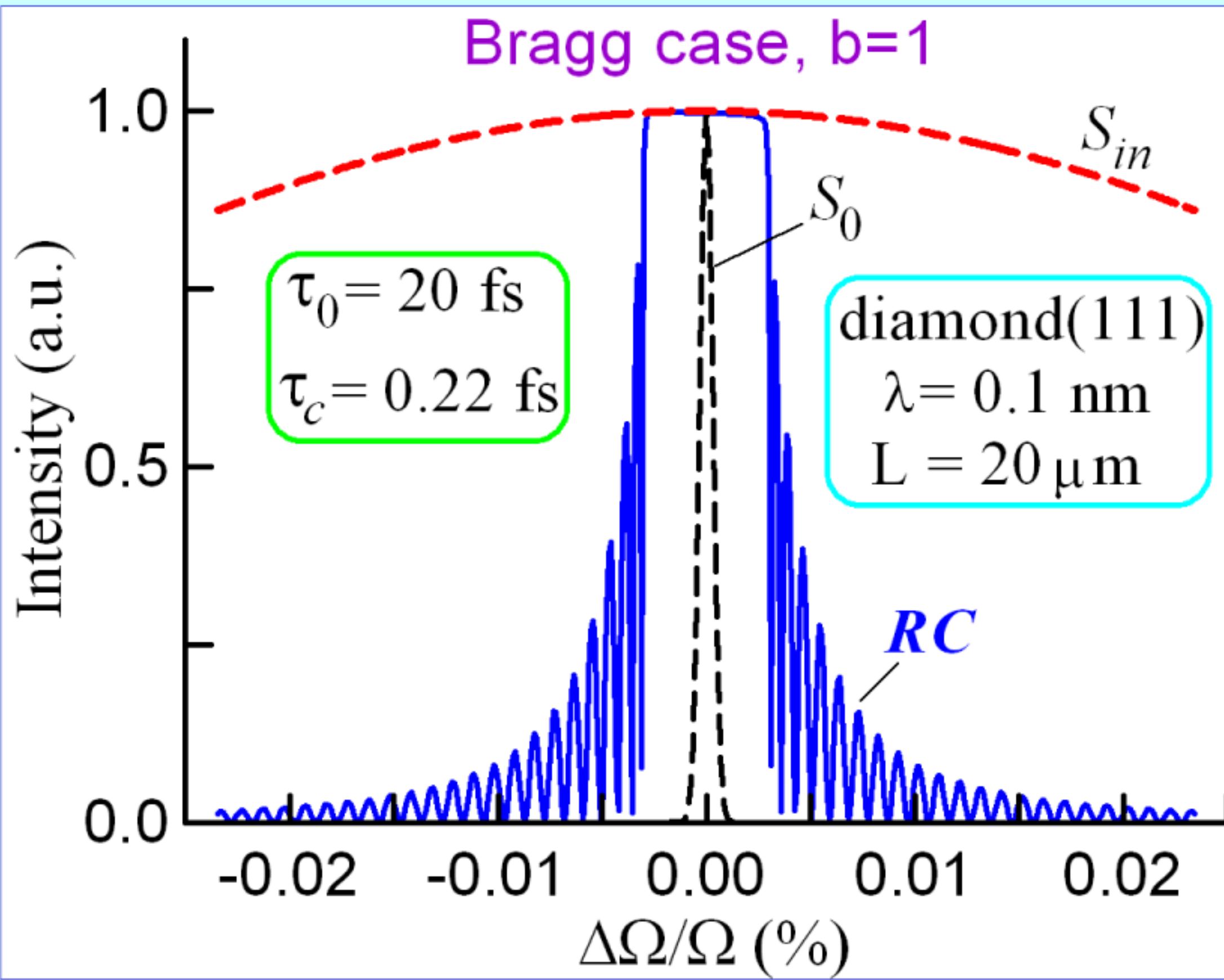
For effective diffraction it is need:

$$\Delta\theta_{difr} < \Delta\theta_B, \quad \Delta\omega/\omega < \Delta\theta_B \operatorname{ctg}\theta_B$$

If $\lambda \sim 1 \text{ \AA}$, $\Delta\theta_B \sim 1 \text{ arcsec} = 5 \mu\text{rad}$, then it must be
 $r_0 \geq 10 \mu\text{m}$, $\tau_0 \geq 10 \text{ fs}$

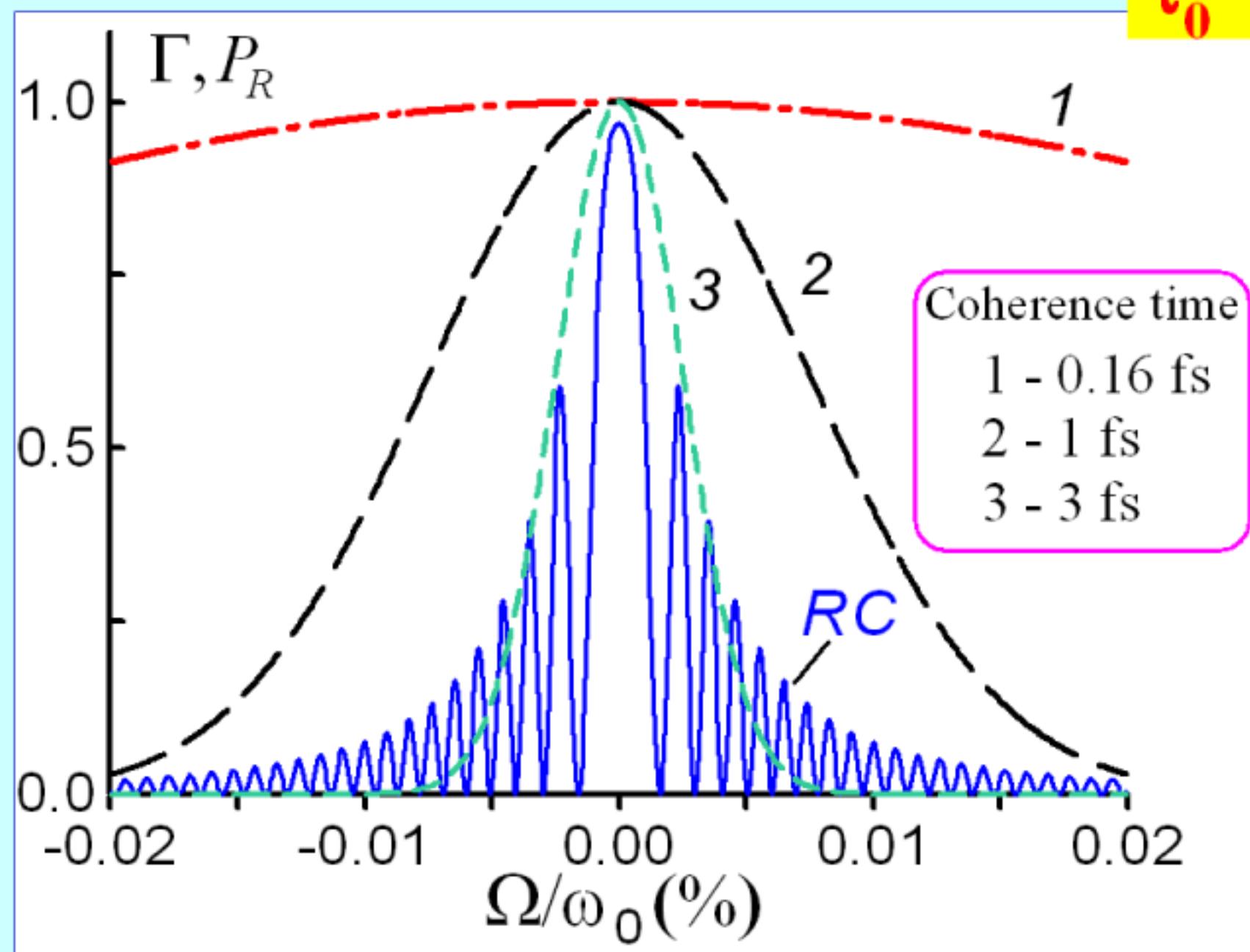
However for XFEL $\tau_0 \sim 0.1 \text{ fs}$!!!

R



Laue case

$\tau_0 = 100 \text{ fs}$

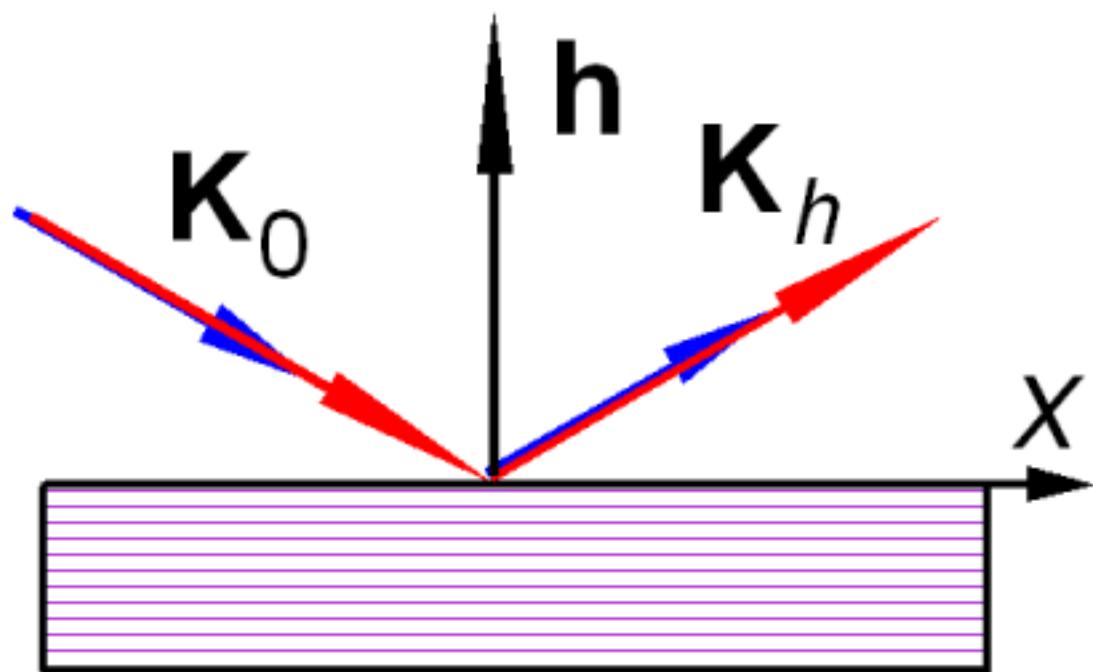


R

Power spectrum density $\Gamma(\Omega)$ of an incident pulse with duration $\tau_0 = 100 \text{ fs}$ and coherence time $\tau_c = 0.16 \text{ fs}$ (1), 1 fs (2) and $\tau_c = 3 \text{ fs}$ (3); RC - a (111) Bragg reflection curve $P_R(\Omega)$ in Laue geometry, **98 μm-thick diamond single** crystal, $\lambda_0 = 0.1 \text{ nm}$.

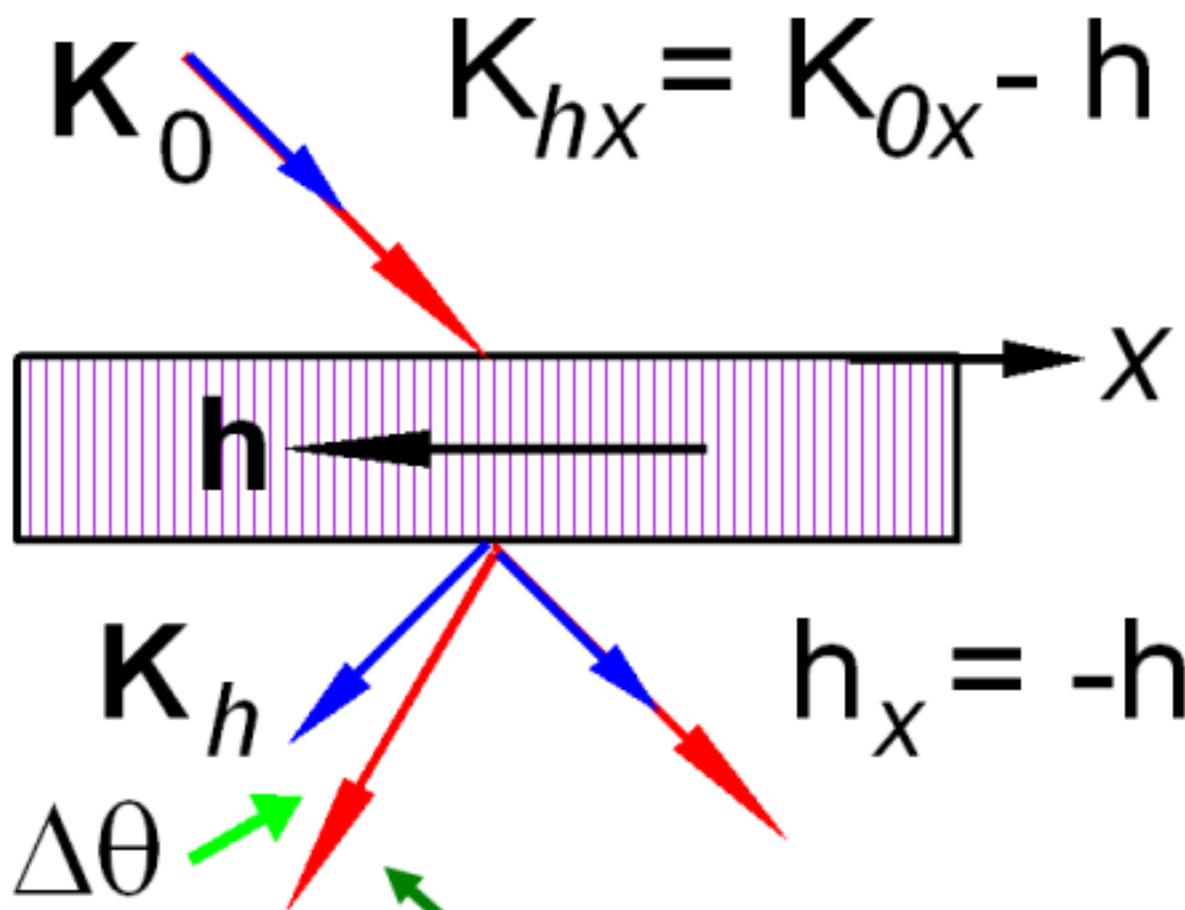
$$\mathbf{k}_h = \mathbf{k}_0 + \mathbf{h}$$

Bragg



$$h_x = 0, \mathbf{K}_{hx} = \mathbf{K}_{0x}$$

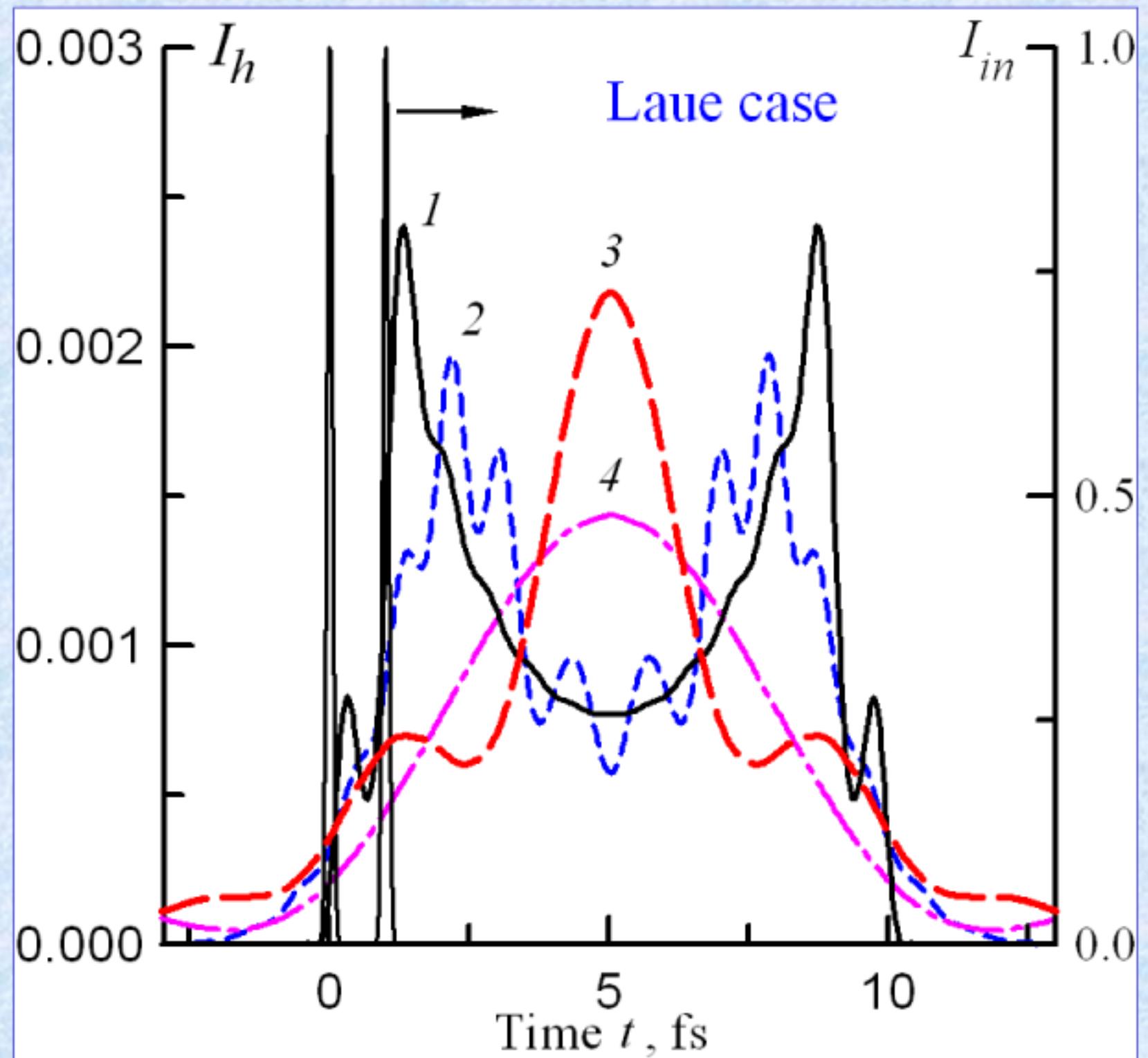
Laue



$$\Delta\theta = -2 \left(\frac{\Delta\omega}{\omega_0} \right) \operatorname{tg} \theta_B$$

Disintegration of the pulse in the space !!!

Laue-reflection of two supershot pulses ("spikes")

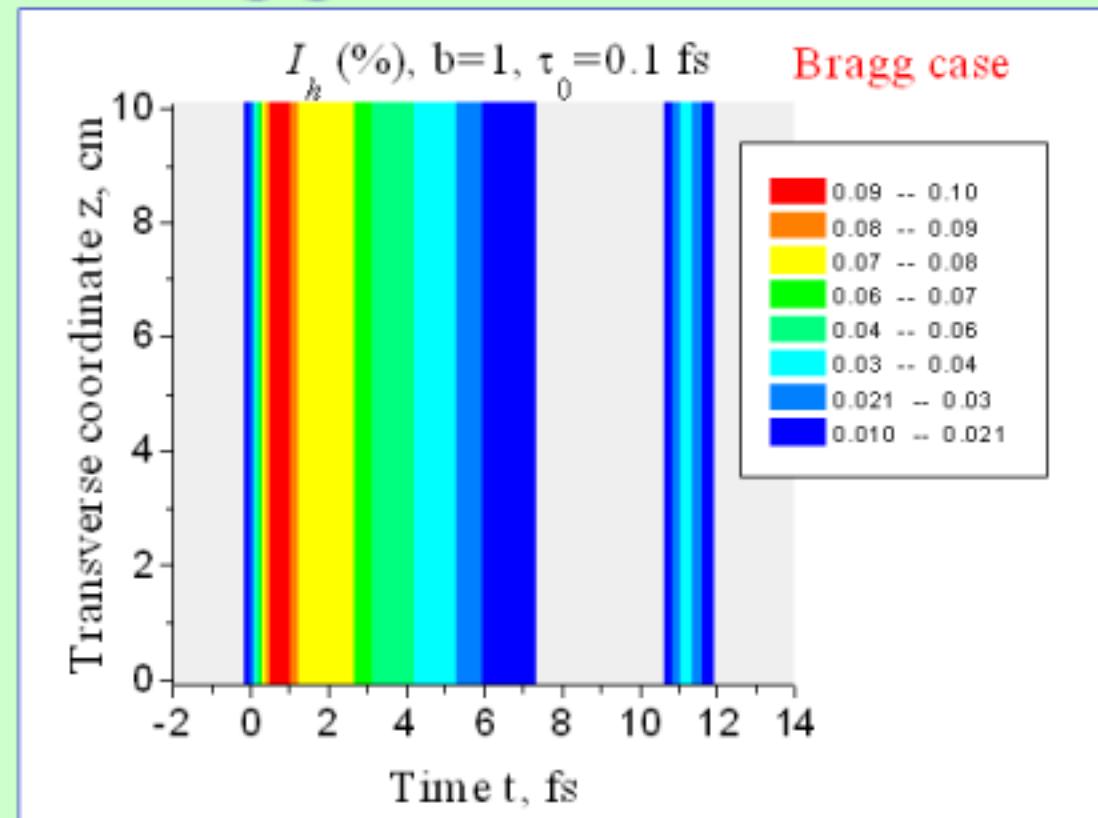


$$\tau_0 = 0.1 \text{ fs}$$

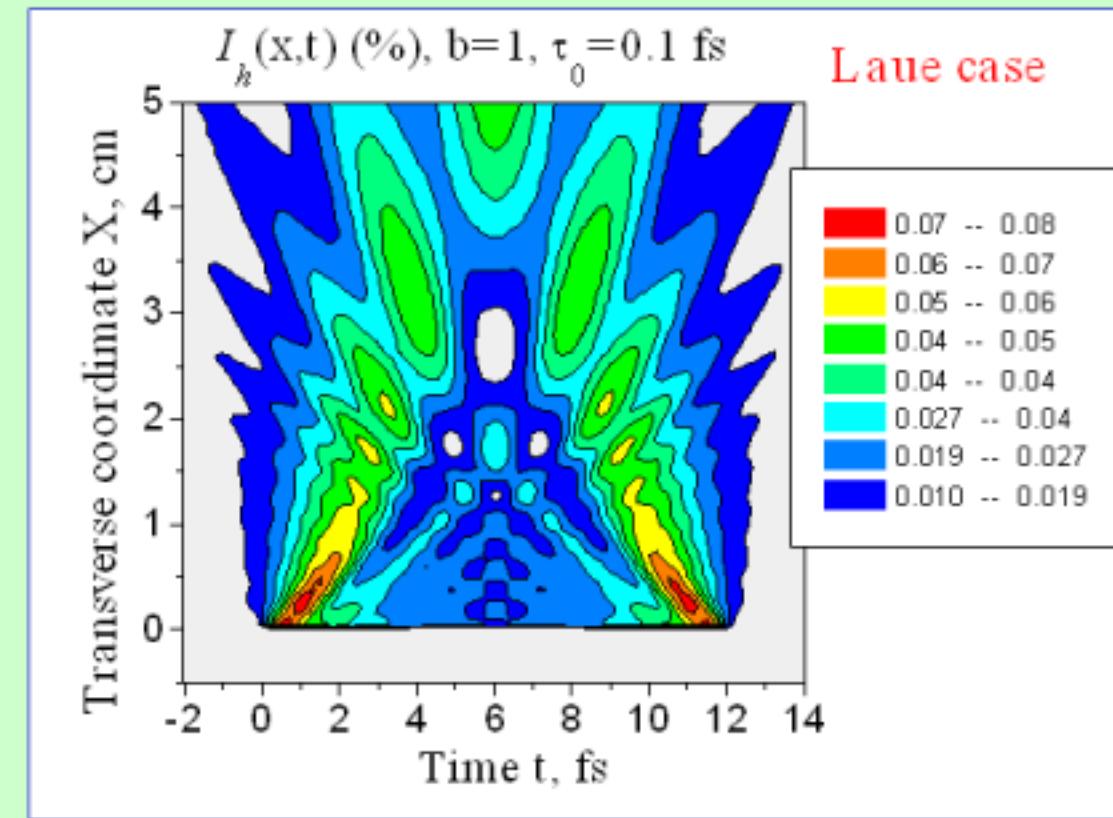
L (cm):
1 - 0
2 - 0.5
3 - 2
4 - 5

$\tau_0 = 0.1 \text{ fs}$, $\Delta t = 1 \text{ fs}$; $\lambda = 0.154 \text{ nm}$, Si(220), $d = 7.73 \mu\text{m}$.

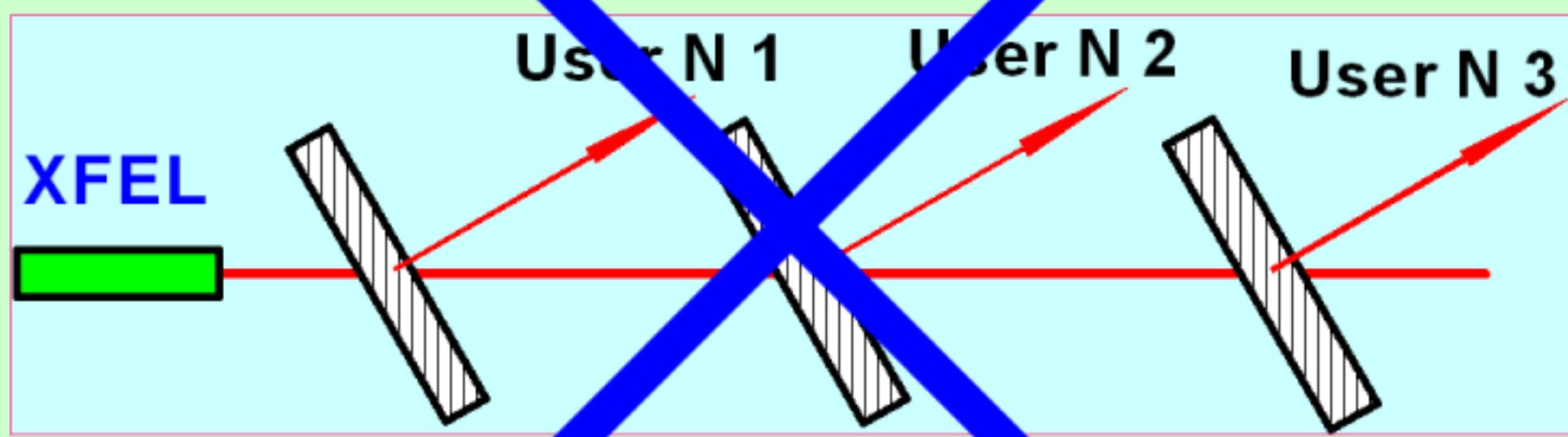
Bragg-case, $b = -1$



Laue-case, $b=1$

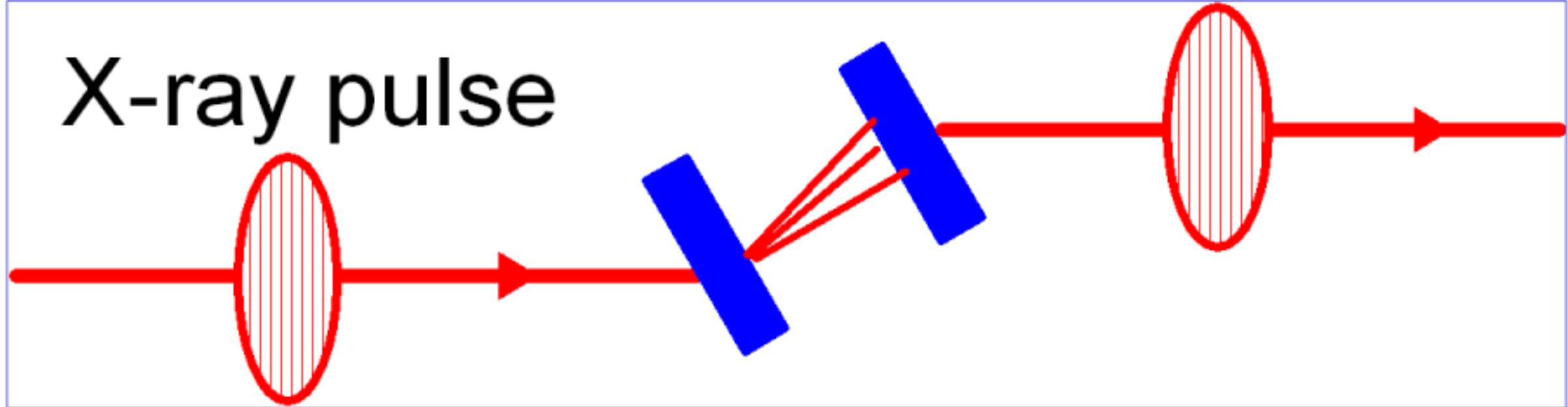


Space-temporal intensity distribution of the reflected pulse;
incident pulse duration is $\tau_0 = 0.1$ fs.



Double-crystal Laue-monochromator

X-ray pulse

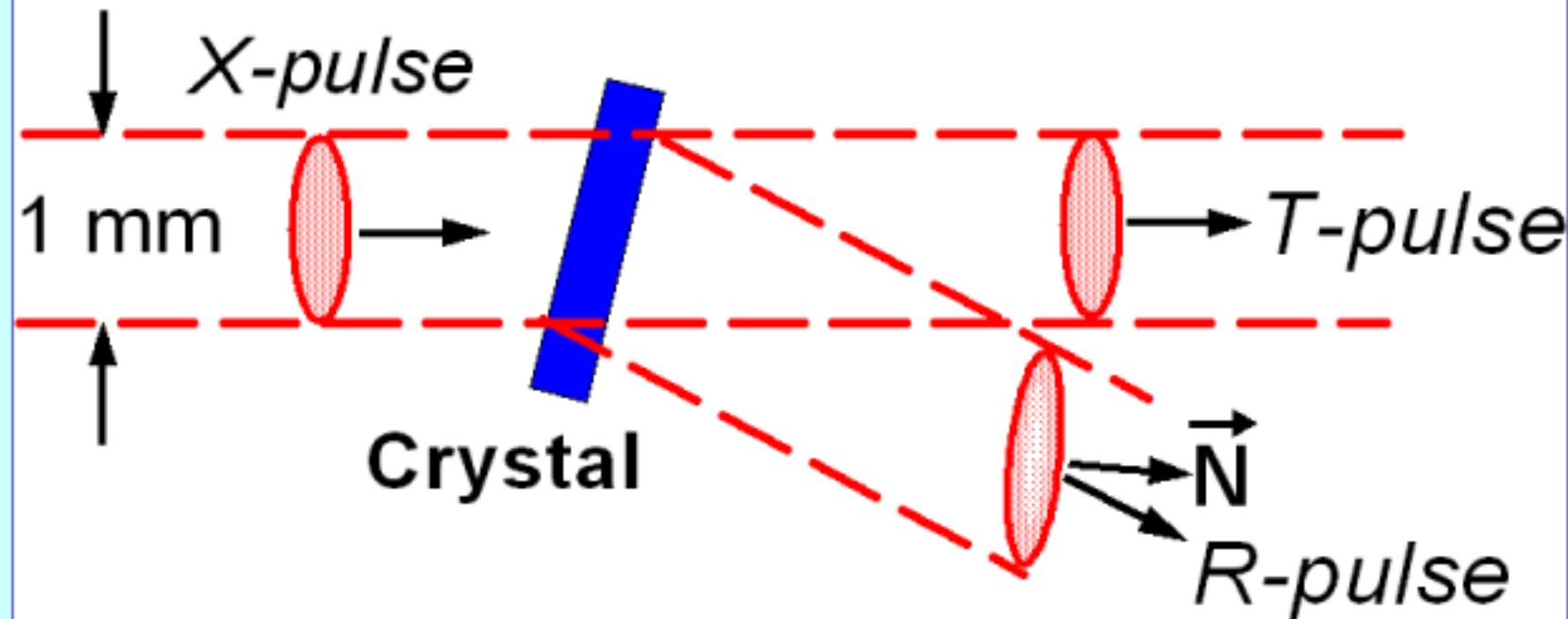


$$A_R(t) = \int_{-\infty}^{\infty} R(\Omega) A(\Omega) \exp[-i\varphi(\Omega, t)] d\Omega$$

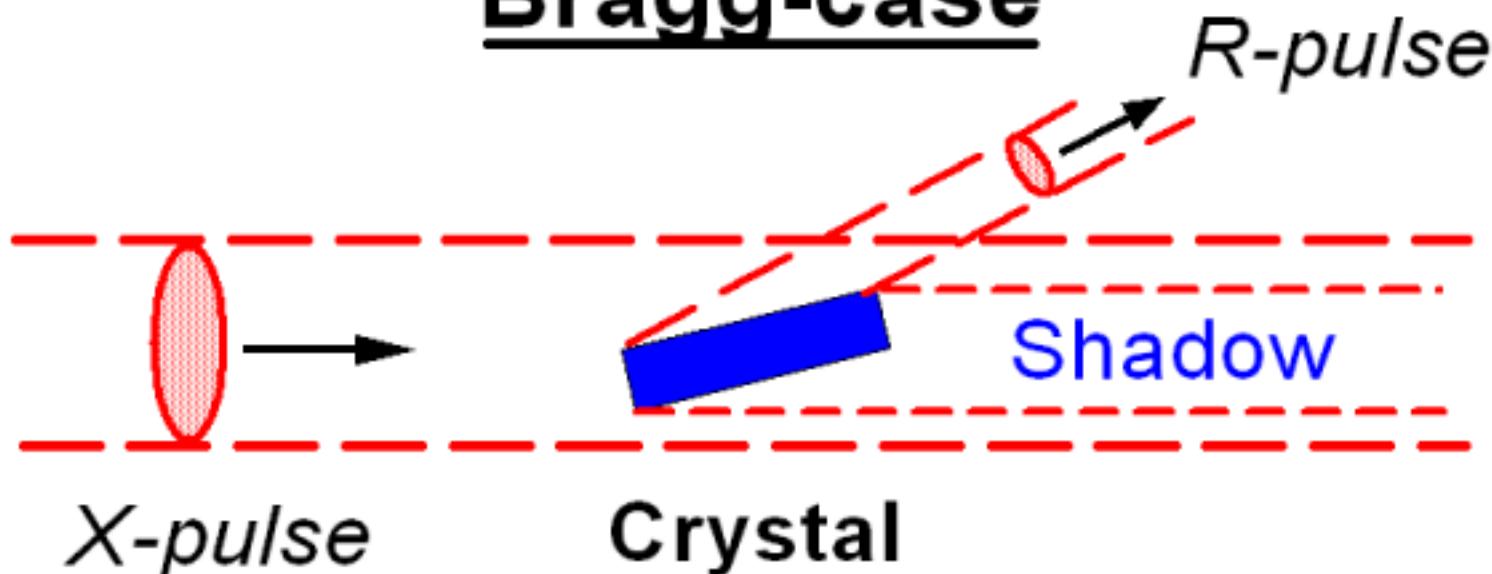
!!

Why is the Laue-geometry ??

Laue-case



Bragg-case



Diamond (111),
 $\lambda = 0.1 \text{ nm}$, $\theta_B = 14^\circ$,
 $L_S \approx 4 \text{ mm}$

Temporal correlation function of the reflected pulse:

$$\Gamma_R(t, \tau) = \langle A_R(t) A_R^*(t + \tau) \rangle$$

Pulse intensity: $I_R(t) = \langle |A_R(t)|^2 \rangle = \Gamma_R(t, 0)$

$$\Gamma_R(t, \tau) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(\Omega, \Omega') R(\Omega) R^*(\Omega') \Phi(\Omega, \Omega'; t, \tau) d\Omega d\Omega'$$

where $g(\Omega, \Omega')$ is a **spectrum correlation function** of the incident pulse:

$$g(\Omega, \Omega') = \langle A(\Omega) A^*(\Omega') \rangle$$

Temporal coherence function of reflected pulse

$$\gamma_R(t, \tau) = \frac{|\Gamma_R(t, \tau)|}{[I_R(t) I_R(t + \tau)]^{1/2}}$$

Simple model for non-stationary SASE radiation with random sub-structure:

The pulse amplitude

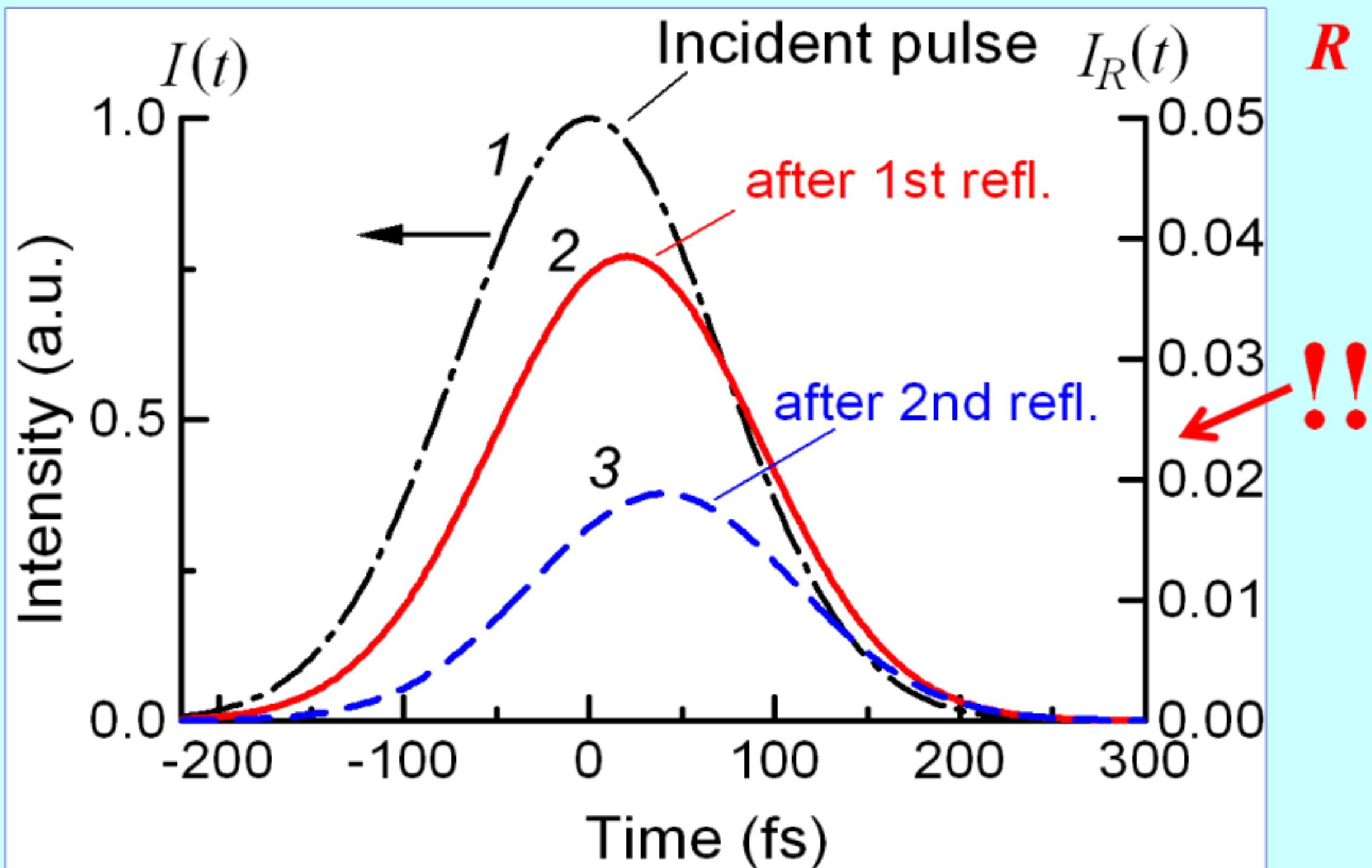
$$A(t) = F(t)a(t),$$

where $F(t)$ is the envelope profile of a pulse and is a regular function of time t ,

$a(t)$ is a **random stationary process**, for which the mean $\langle a(t) \rangle = 0$, intensity $\langle a(t)a^*(t) \rangle = 1$ and correlation function $\gamma(\tau) = \langle a(t)a^*(t + \tau) \rangle$ are time-independent.

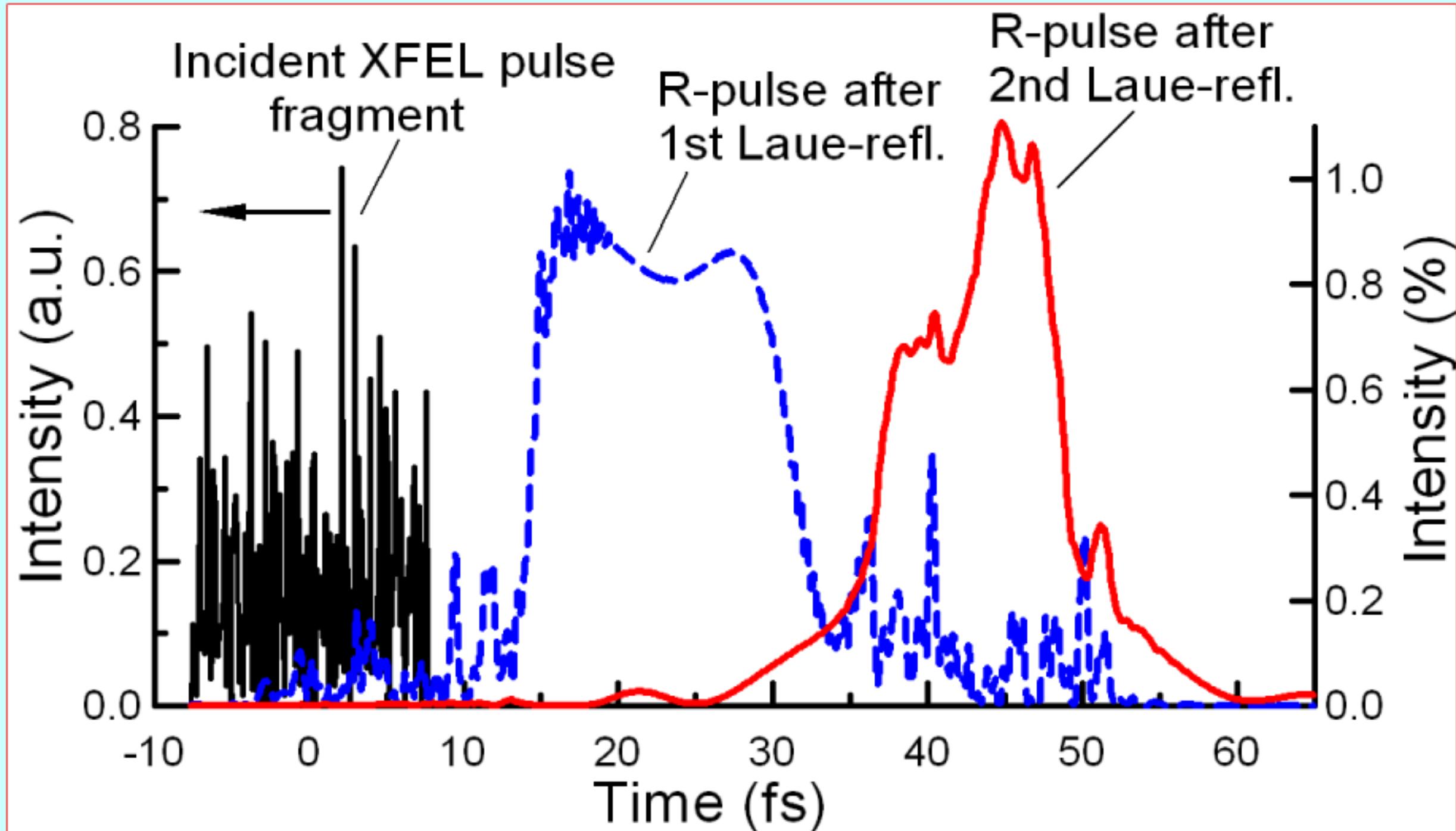
For such a random signal $\langle a(\Omega)a^*(\Omega) \rangle = G(\Omega)\delta(\Omega - \Omega)$, where, according to the Wiener–Khinchin theorem, the signal spectral density is

$$G(\Omega) = (1/2\pi) \int_{-\infty}^{\infty} \gamma(\tau) \exp(-i\Omega\tau) d\tau.$$



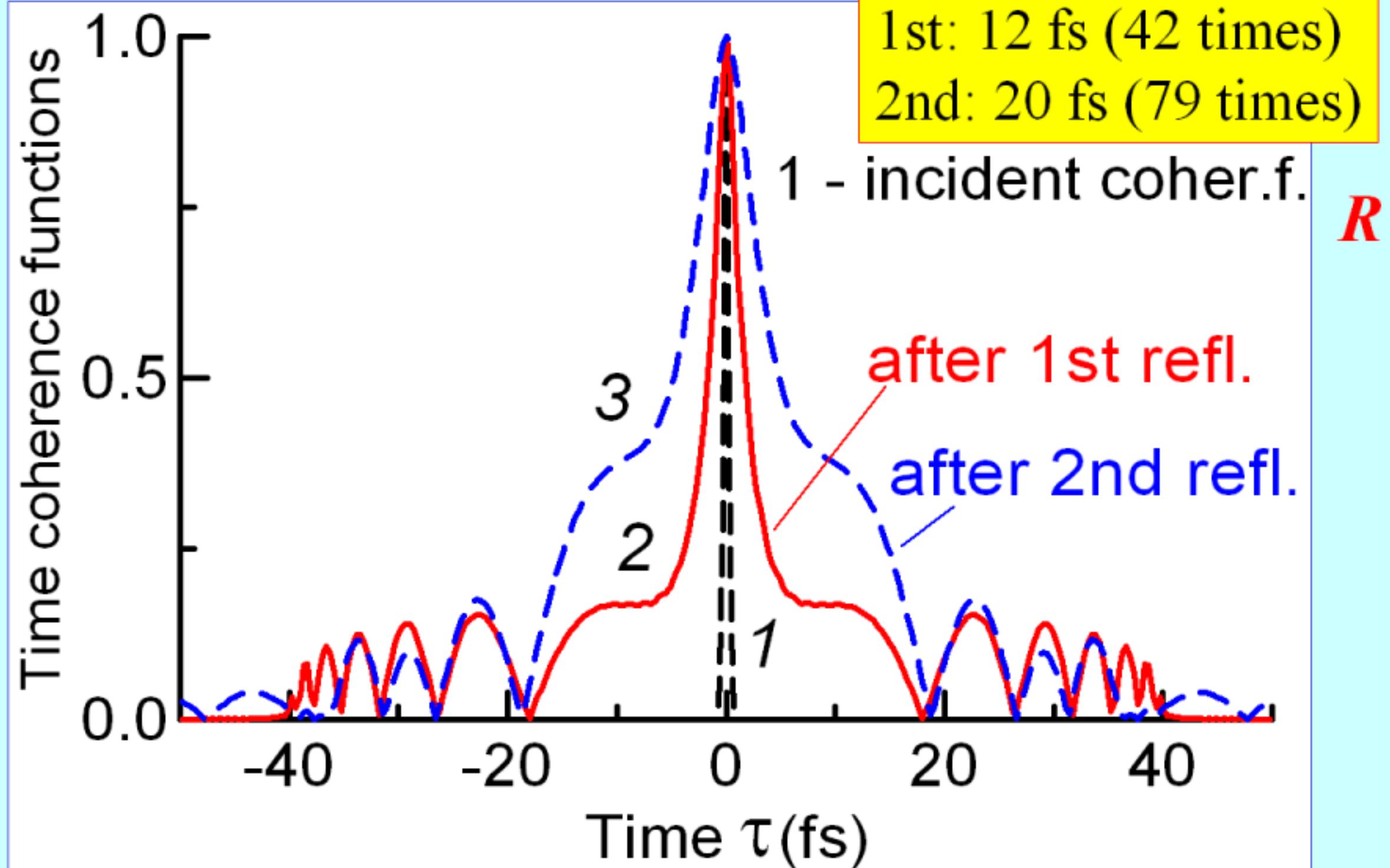
Bragg diffraction in **Laue geometry** of an incident pulse (I) with duration $\tau_0 = 100$ fs and coherence time $\tau_C = 0.16$ fs after the first (2) and the second (3) monochromator crystals, diamond(111).

Two-fold Laue-reflection of the XFEL pulse fragment



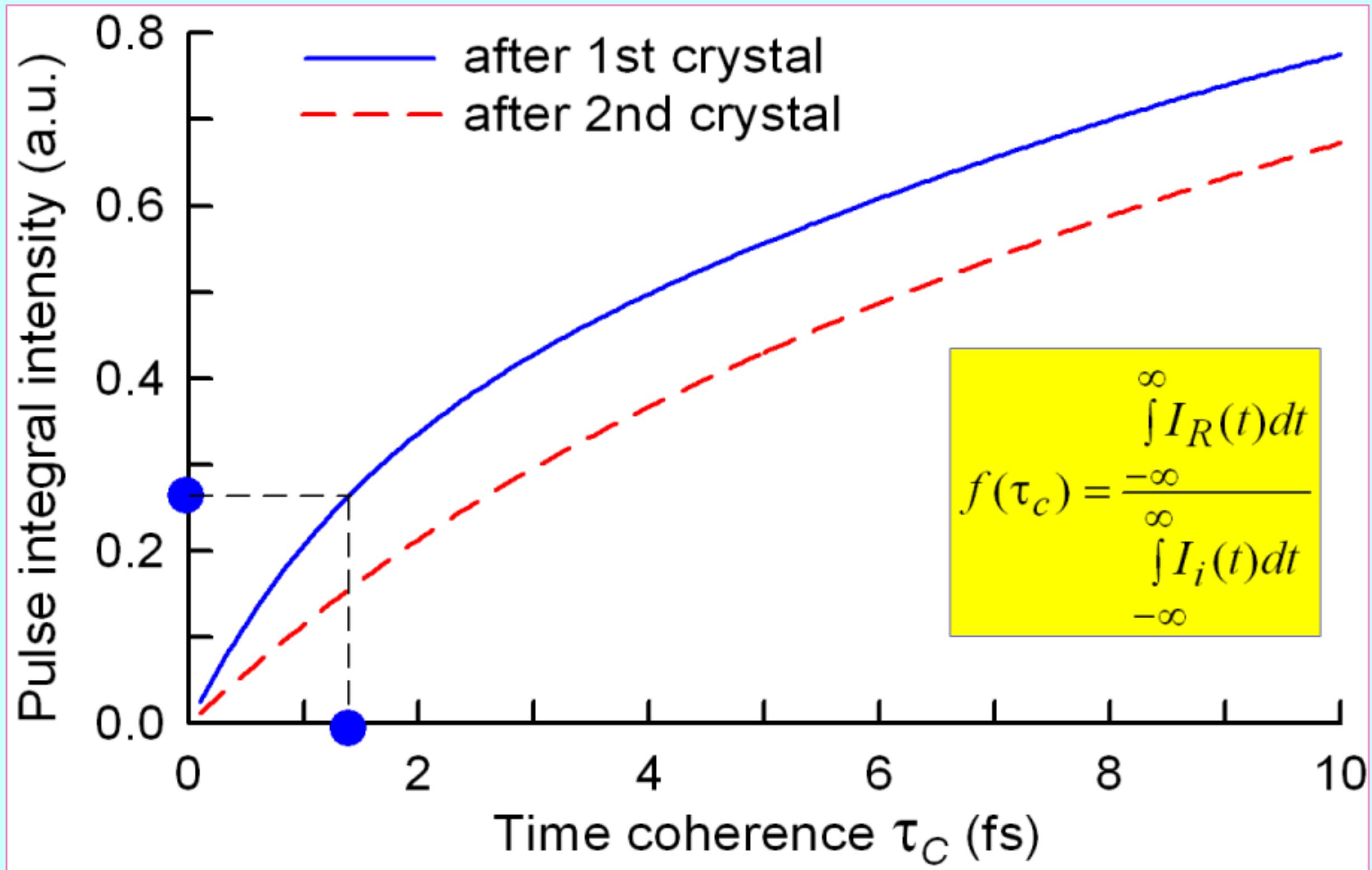
Diffraction reflection of XFEL pulse fragment (by M.Yurkov calc.)
on two crystals in the Laue-geometry; crystals thickness is 98 μm .

Incident: 0.3 fs
1st: 12 fs (42 times)
2nd: 20 fs (79 times)



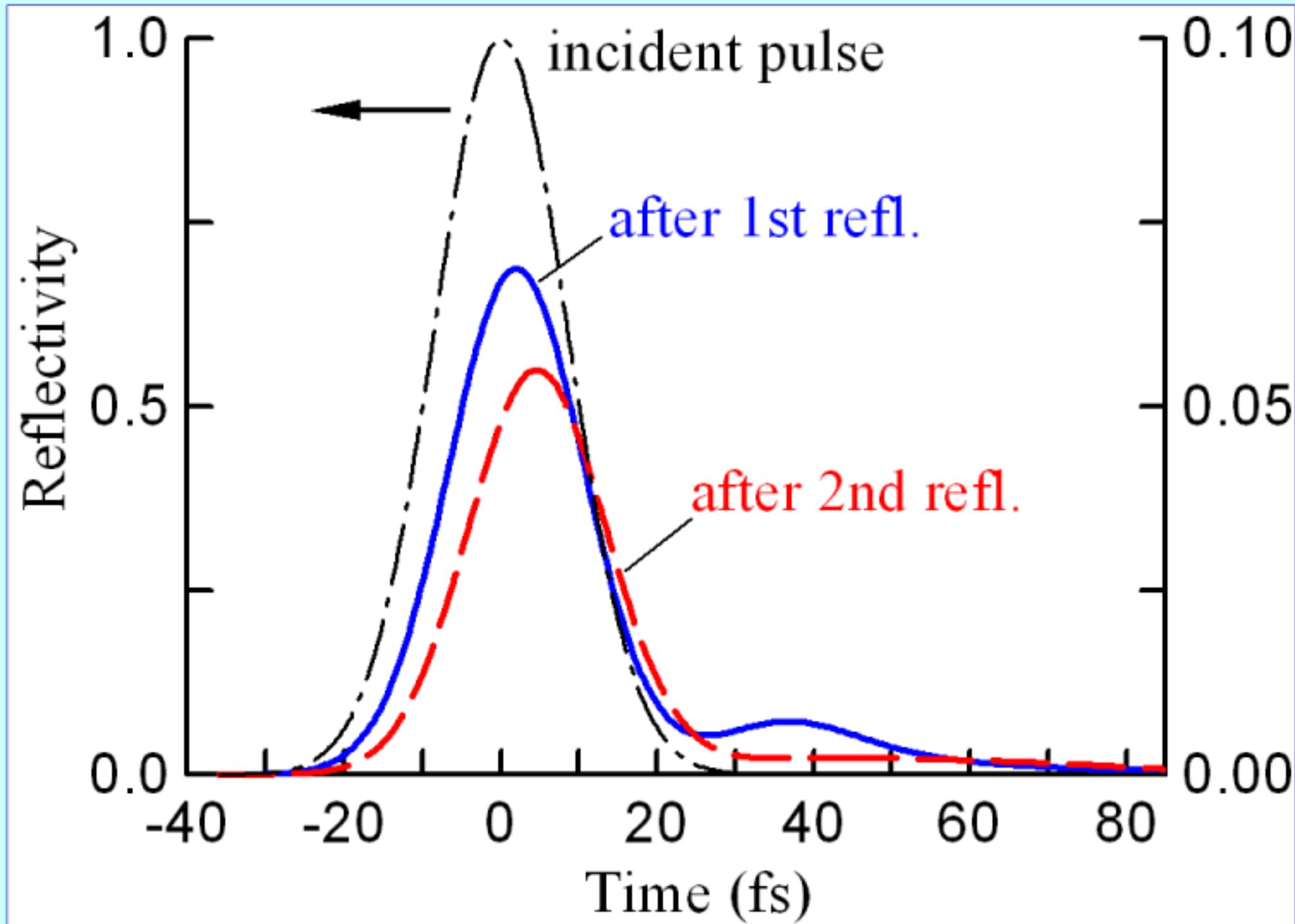
Time coherence functions of an incident pulse $\gamma(\tau)$ (1) and the diffracted pulse $\gamma_R(t_{max}, \tau)$ after the 1st (2) and the 2nd (3) Laue-crystals.

Simple method of coherence time measurement



Bragg case, diamond(111), $b = 1$

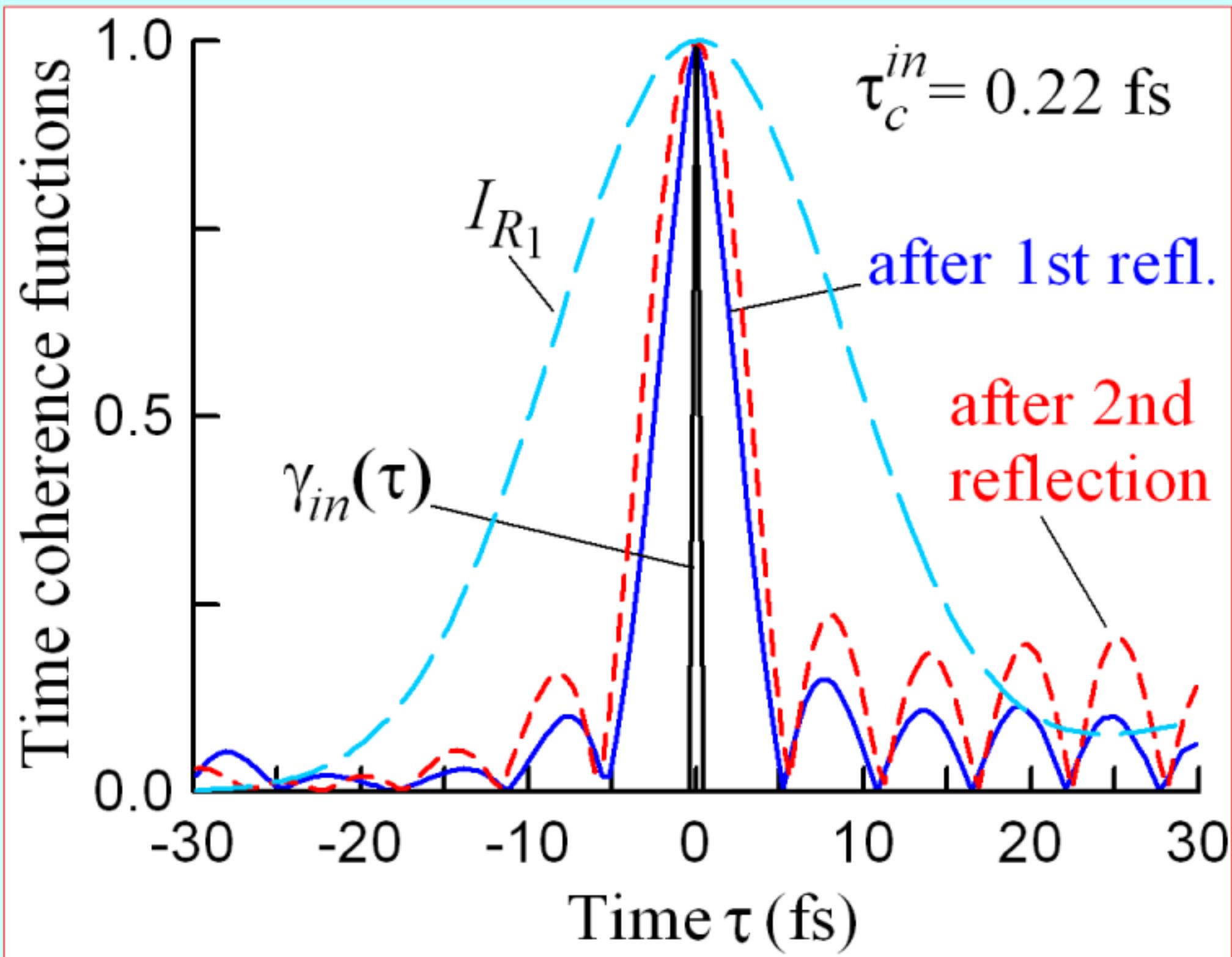
R



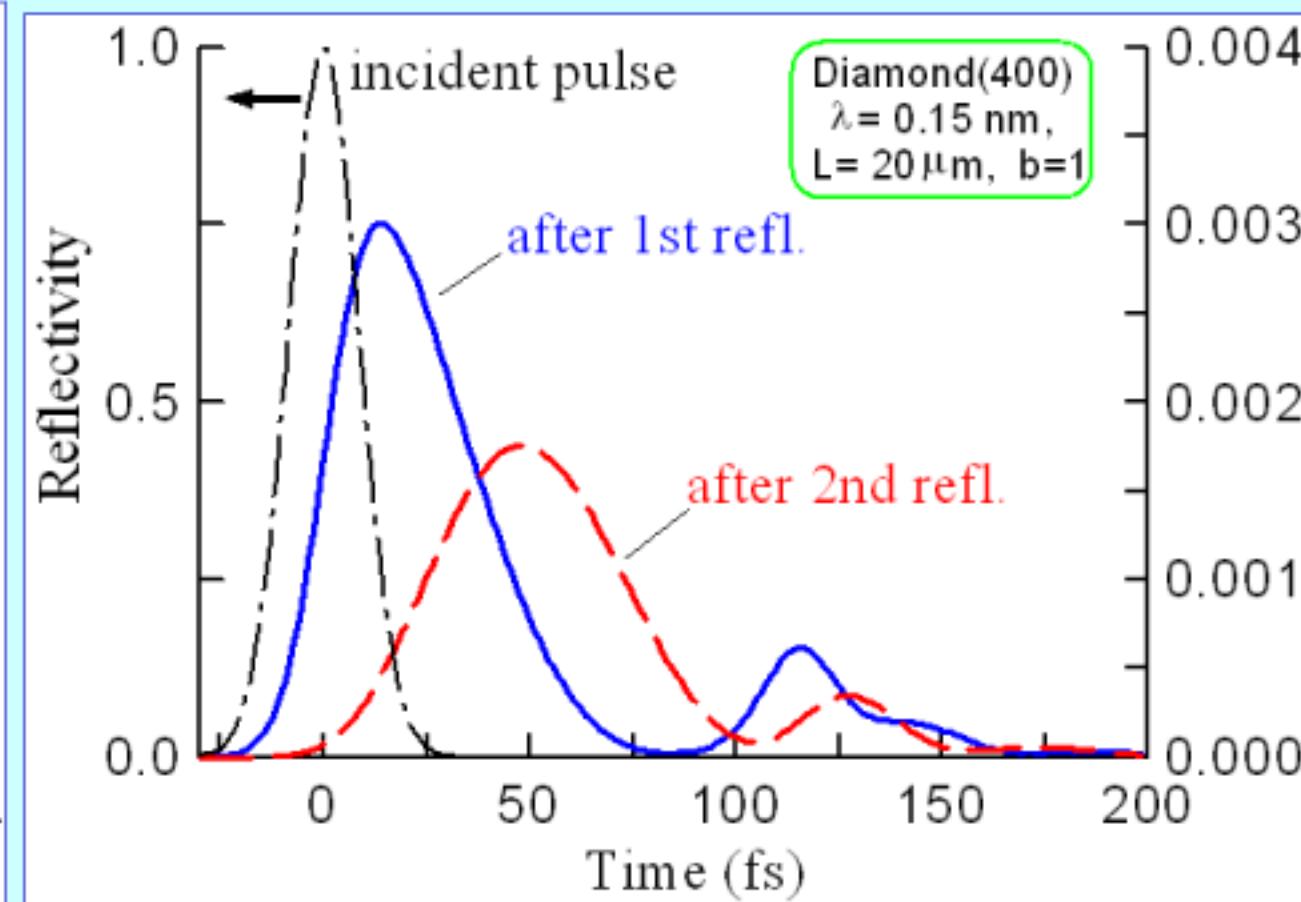
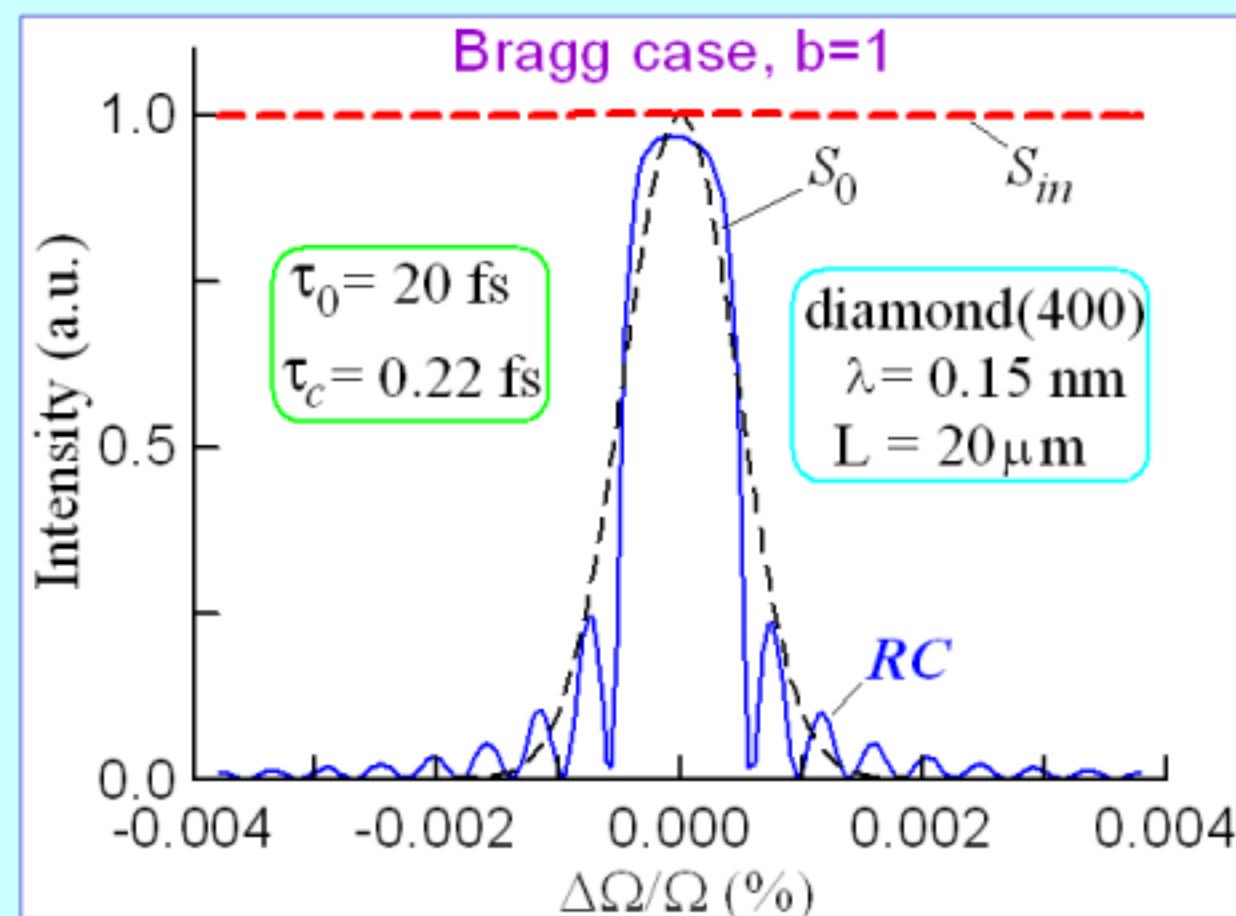
Crystal thickness $L = 20 \mu\text{m}$, $\lambda = 0.1 \text{ nm}$, $\tau_0 = 20 \text{ fs}$, $\tau_c = 0.22 \text{ fs}$.

Time coherence functions
Bragg case, diamond(111), $b = 1$

R

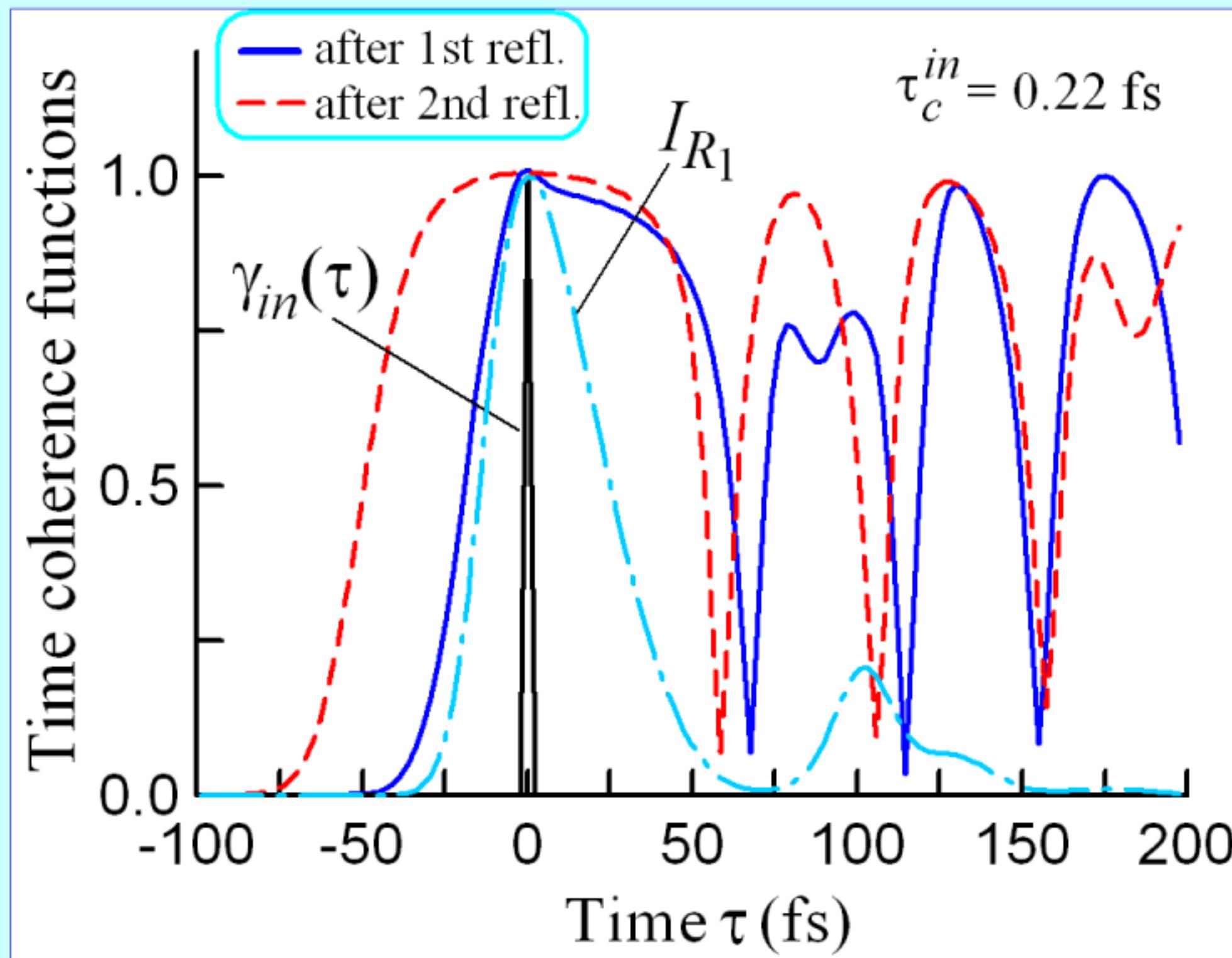


Bragg case, diamond(400), $b = 1$, R
 $L = 20 \mu\text{m}$, $\lambda = 0.15 \text{ nm}$, $\tau_0 = 20 \text{ fs}$, $\tau_c = 0.22 \text{ fs}$.

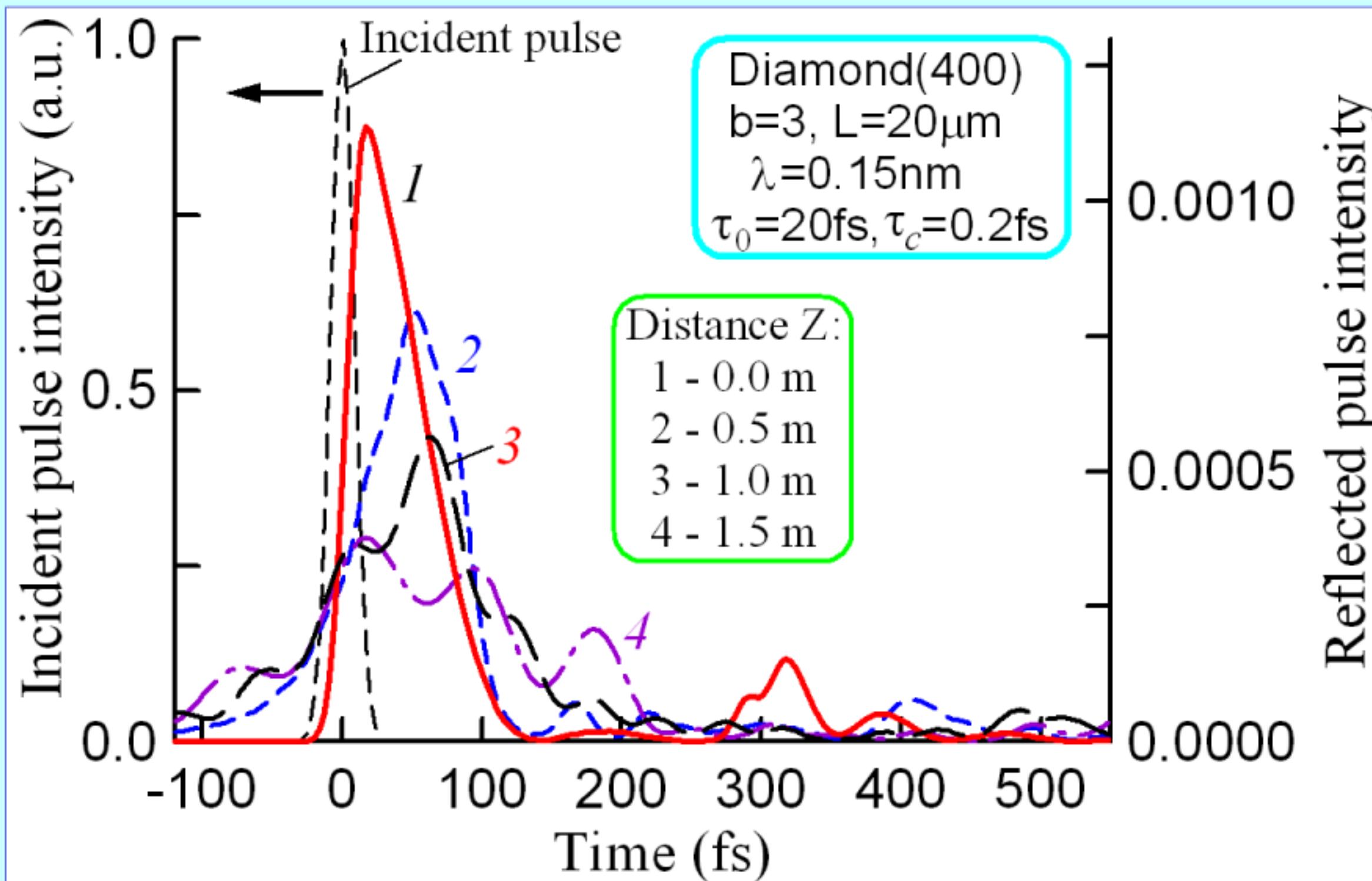


Time coherence functions

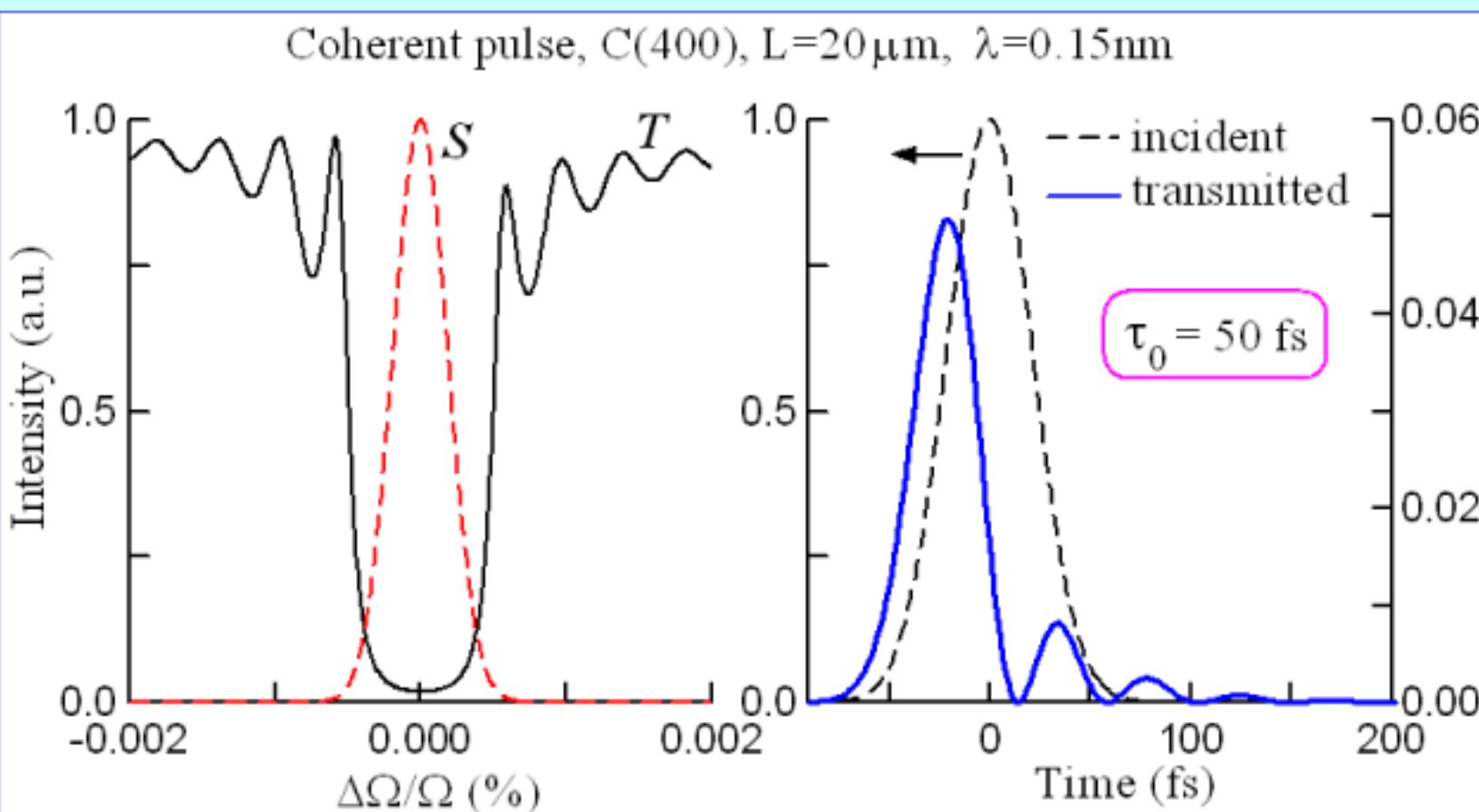
Bragg case, diamond(400), $b = 1$



Non-symmetrical Bragg reflection



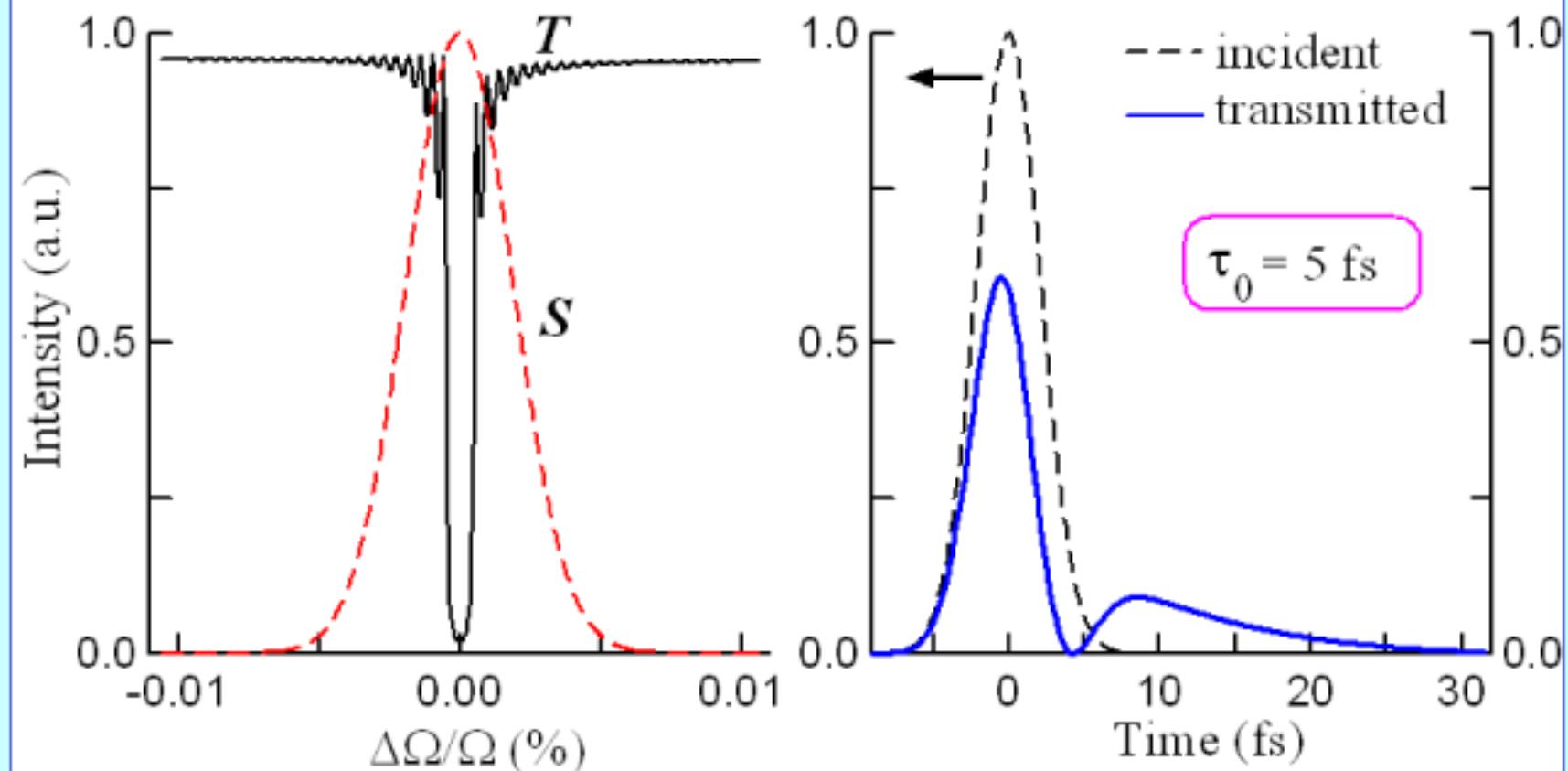
Coherent pulse, C(400), L=20 μ m, $\lambda=0.15$ nm



**Pulse transmission
in Bragg geometry**

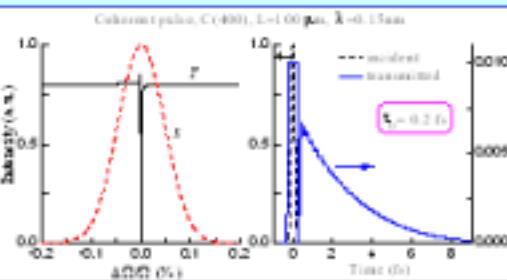
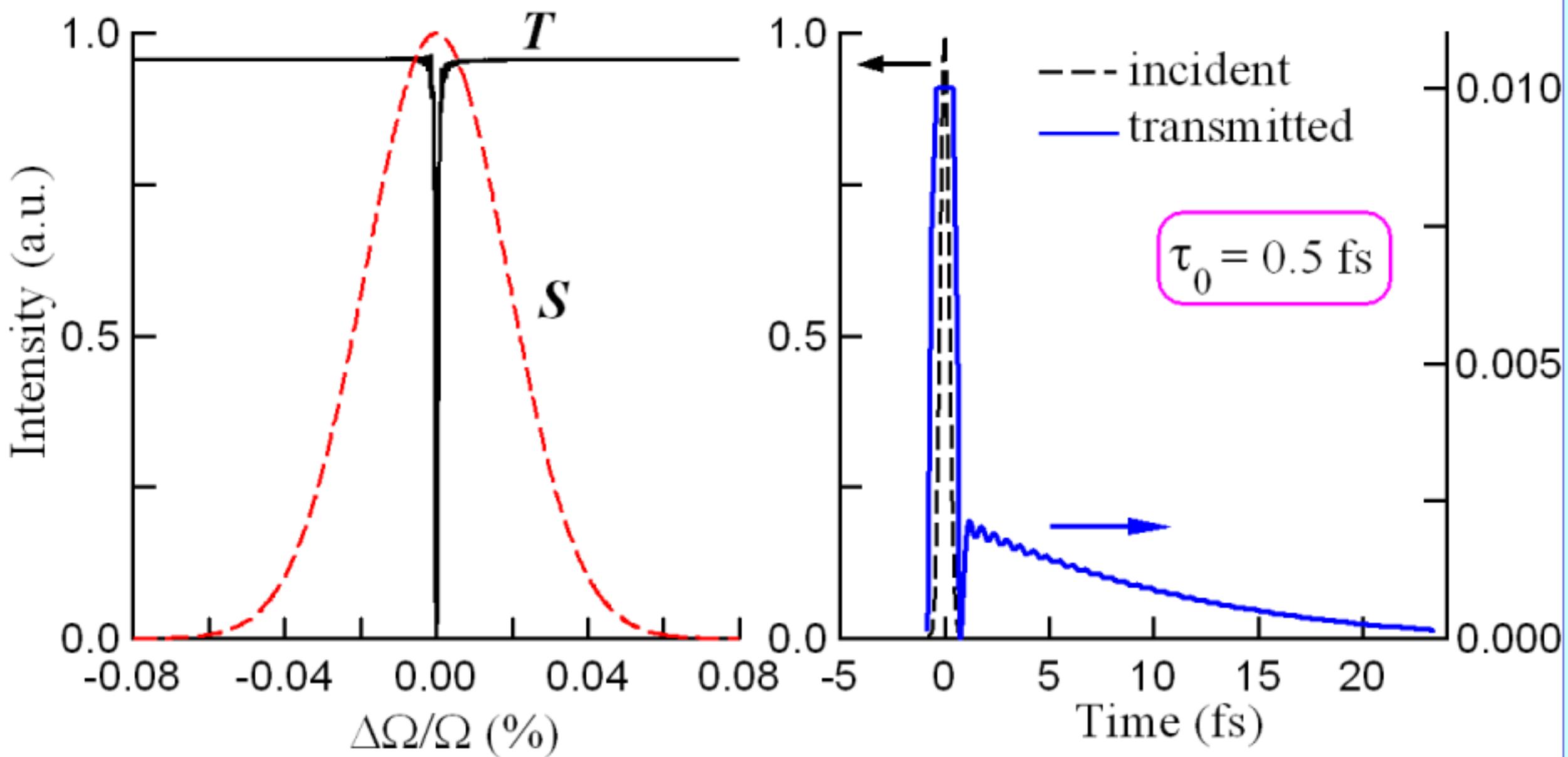
T

Coherent pulse, C(400), L=20 μ m, $\lambda=0.15$ nm

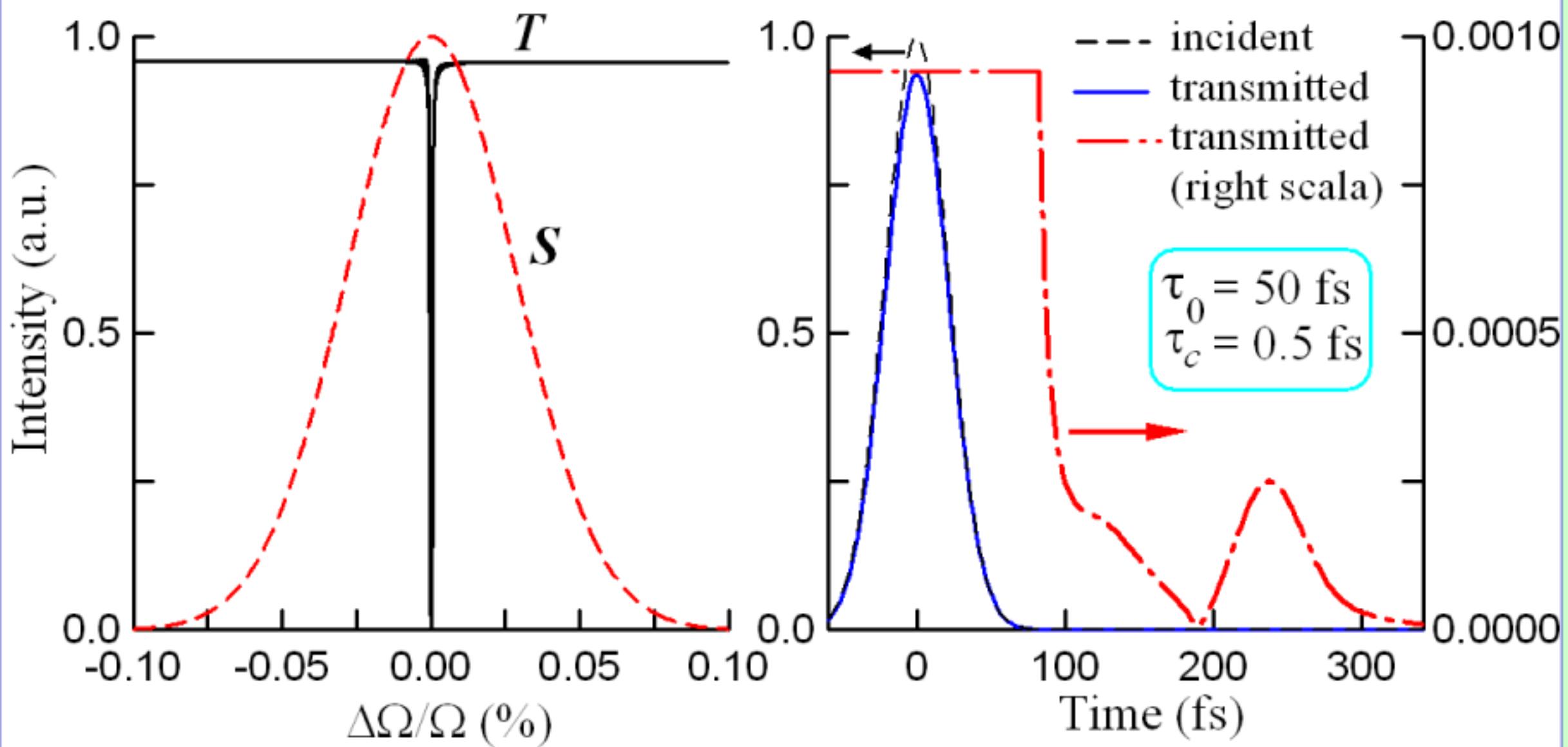


T

Coherent pulse, C(400), L=20 μ m, $\lambda=0.15\text{nm}$



Noncoherent pulse, C(400), L=20 μ m, $\lambda=0.15\text{nm}$



Bandwidth down to 10^{-5}

T

Заключение:

1. На расстояниях, реализуемых в EuroXFEL, плохая временная когерентность импульса не влияет на его пространственную когерентность
2. Отражение от двукратного Лауз-монохроматора приводит к уменьшению интенсивности импульса на два порядка без искажения формы импульса
3. Форма функции временной когерентности меняется существенным образом, интегральное время когерентности увеличивается почти на 2 порядка
4. Предложен простой метод измерения времени когерентности по данным интегральных интенсивностей падающего и отраженного импульсов

Спасибо за внимание



МГУ



XFEL