

Effect of the Thermal Heating of a Crystal on the Diffraction of Powerful Pulses of a Free-Electron X-Ray Laser



Vladimir Bushuev

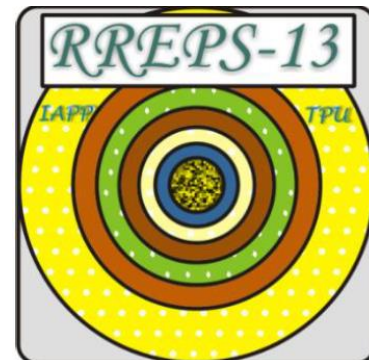
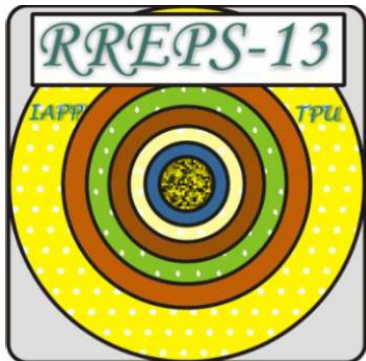
*M.V. Lomonosov Moscow State University
Moscow, Russia*

e-mail: vabushuev@yandex.ru



**X International Symposium
"Radiation from Relativistic Electrons
in Periodic Structures" – RREPS-13**

**Armenia
Yerevan – Sevan
September 23-27, 2013**



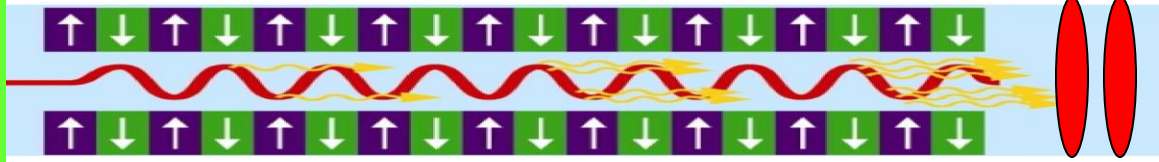
Short plan:

- 1. A few words about X-ray Free-Electron Laser (XFEL) and parameters of the pulses**
- 2. Temperature dependences of the coefficients of specific heat capacity, the heat conductivity, and the linear thermal expansion coefficient**
- 3. Thermal conductivity equation**
- 4. Spatio-temporal distribution of the reflected and transmitted pulse intensities after diffraction of XFEL powerful pulses**

Basic principles of X-ray free electron lasers³

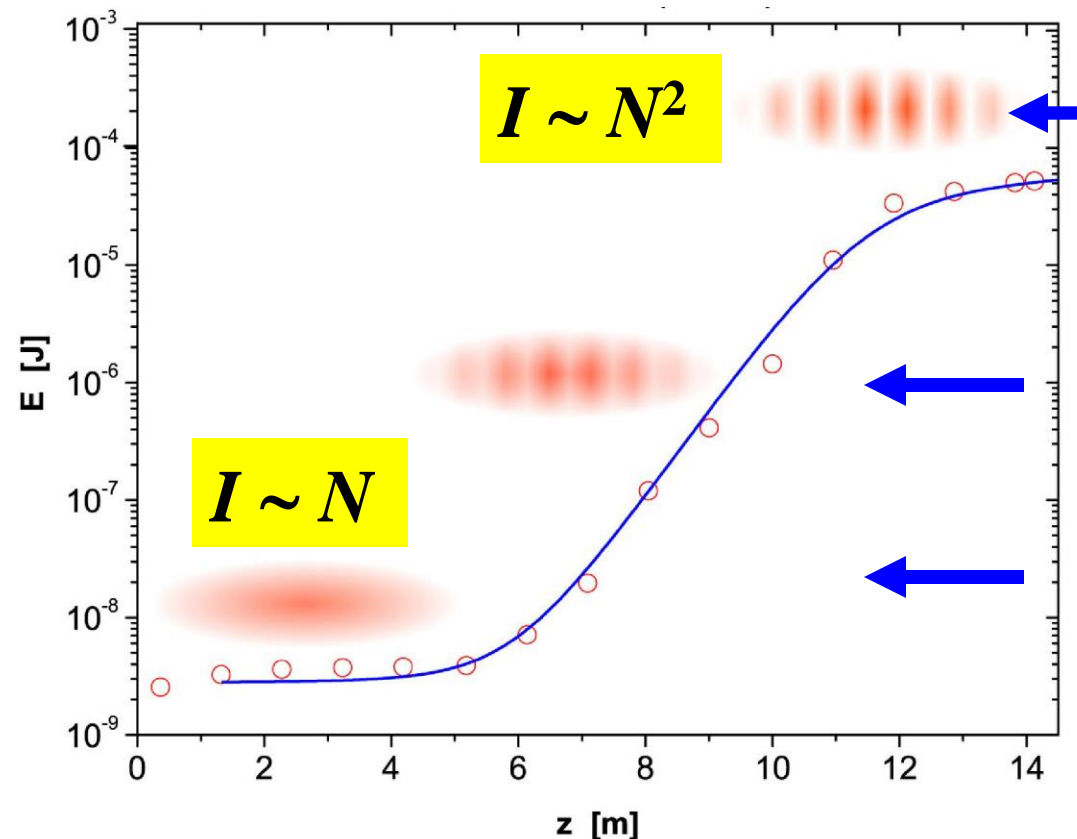
Long undulator (15-150 m)

Electron beam
 $E_{el} \sim 10-15$ GeV



**XFEL
pulses**

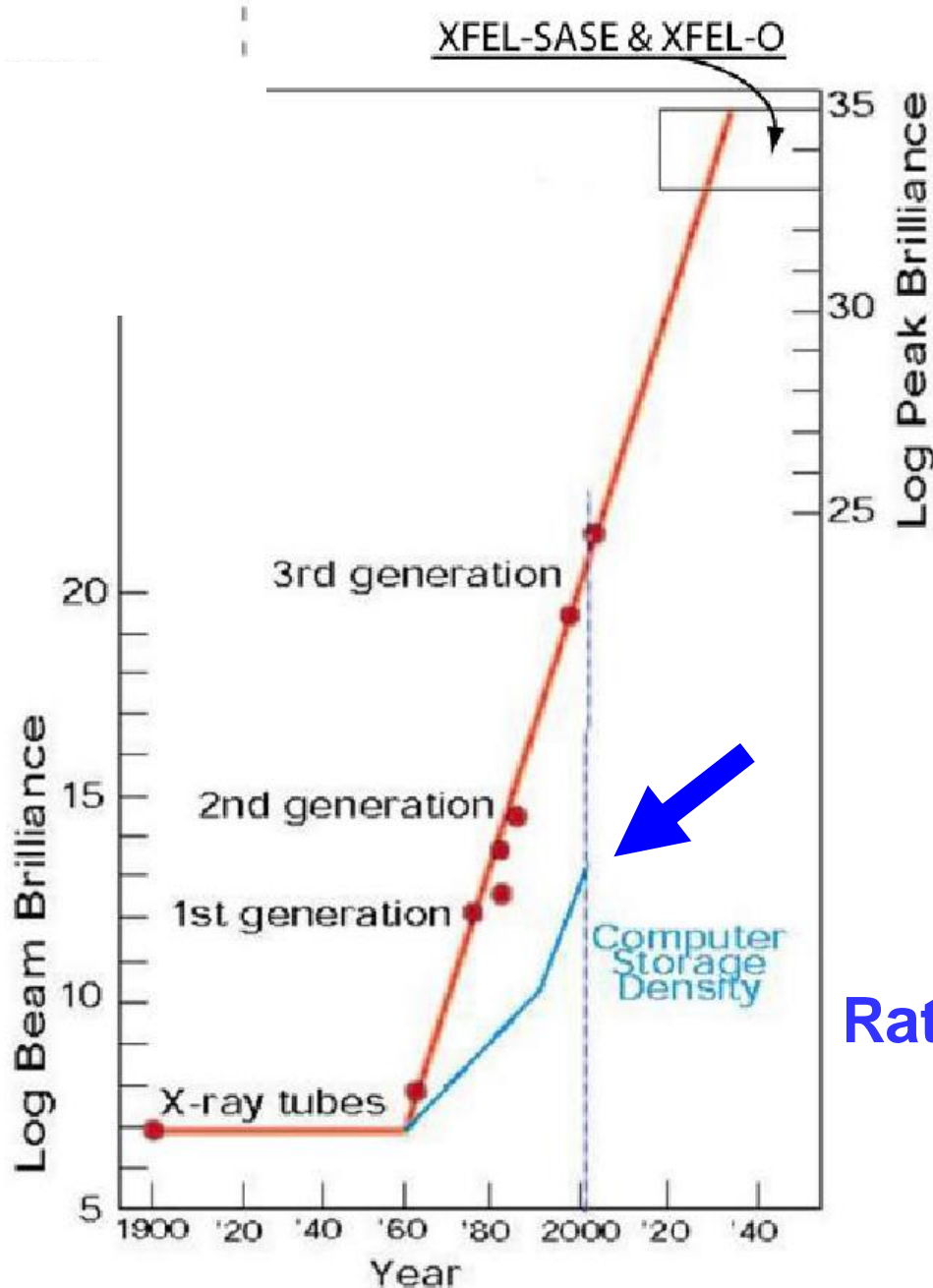
Self-Amplified Spontaneous Emission (SASE)



3. With complete micro-bunching all electrons radiate in phase. This leads to a radiation power growth as N^2 .

2. The shot noise of the electron beam is amplified to complete micro-bunching.

1. All N electrons can be treated as individually radiating charges, and the resulting spontaneous emission is proportional to N .



X-ray free electron laser starting from the shot noise in the electron beam has been proposed by Derbenev, Kondratenko, and Saldin (1979, 1982); and also by Bonifacio, Pellegrini and Narducci (1984).

Ratio of XFEL and SR brilliances:

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



Hard X-ray (SASE1 and SASE2) FEL radiation

typical main parameters

Radiation wavelength	0.1 nm	
Bunch charge	0.02 nC	1 nC
Pulse duration	10 fs	100 fs
Source size (FWHM)	29 μm	49 μm
S. divergence (FWHM)	1.9 μrad	1.3 μrad
Spectral bandwidth	1.9×10^{-3}	1.0×10^{-3}
Coherence time	0.13 fs	0.23 fs
Degree of the transverse coherence	0.95	0.71
Photons/pulse	0.3×10^{11}	6.4×10^{11}
Pulse energy	58 μJ	1260 μJ

Low

High !!

General time structure of the EU XFEL

Hard X-ray (SASE1 and SASE2)

Wavelength: 0.05 – 0.16 nm

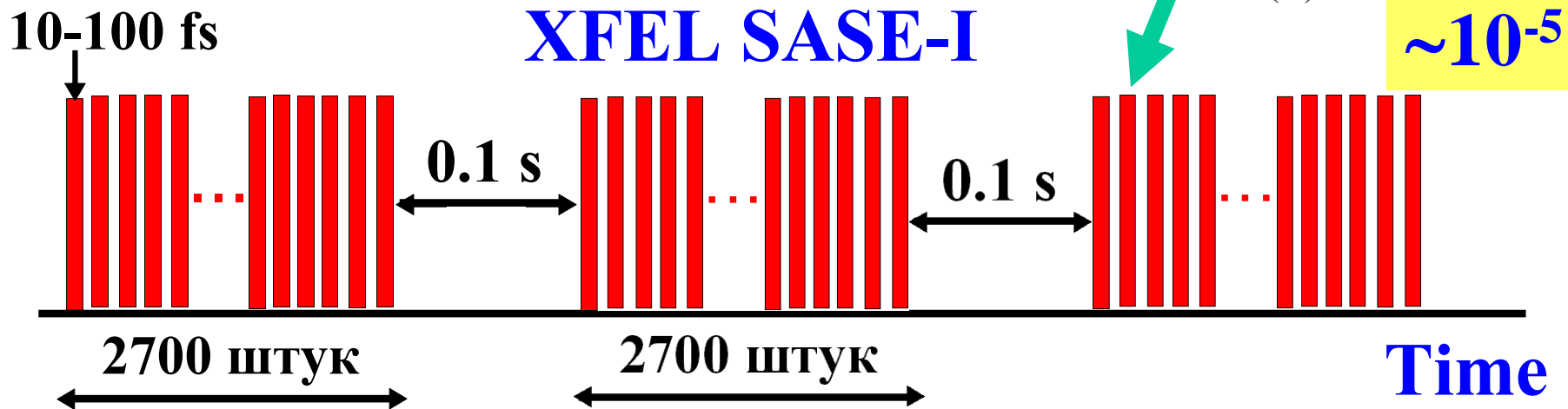
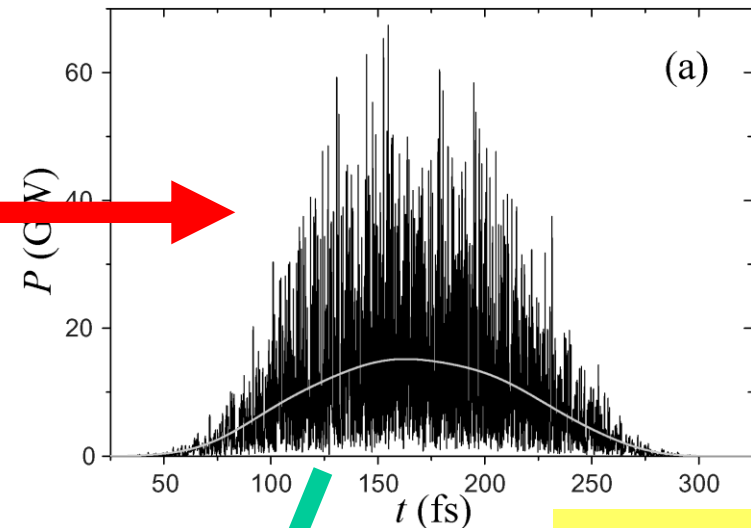
Bunch charge: 0.02 – 1 nC !!

Photons/pulse: $(0.1 - 20) \times 10^{11}$

Pulse Energy: 20 – 2500 μJ

Power: 60 W/cm² – 80 kW/cm²

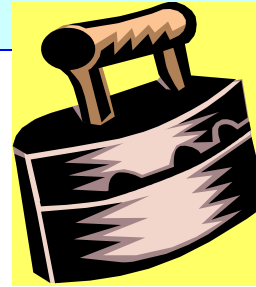
$$\Delta E/E \approx 10^{-3}$$



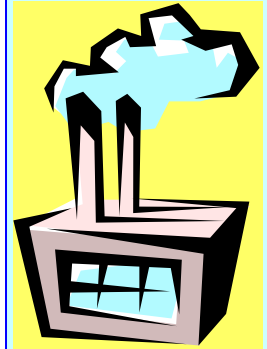
Linac Coherent Light Source (LCLS) – одиночные импульсы, 120 Гц

...For comparison:

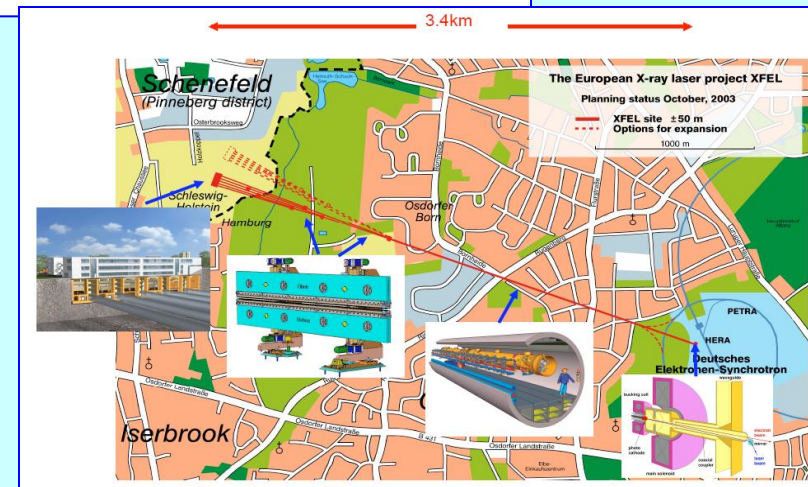
1. Iron - 5 W/cm^2



2. Thermal elements
on atomic stations - 200 W/cm^2



3. XFEL - $3\text{-}10 \text{ kW/cm}^2$



There are three problems:

1. How powerful XFEL pulses heat up a crystal (in space and in time)?
2. How this heating influences on the diffraction of pulses?
(monochromatisation, self-seeding)
3. On what distance we should place a crystal ?

**Main
problem:**



$$I, T, d, \theta_B = f(\mathbf{r}, t)$$

Simple estimations (for diamond):

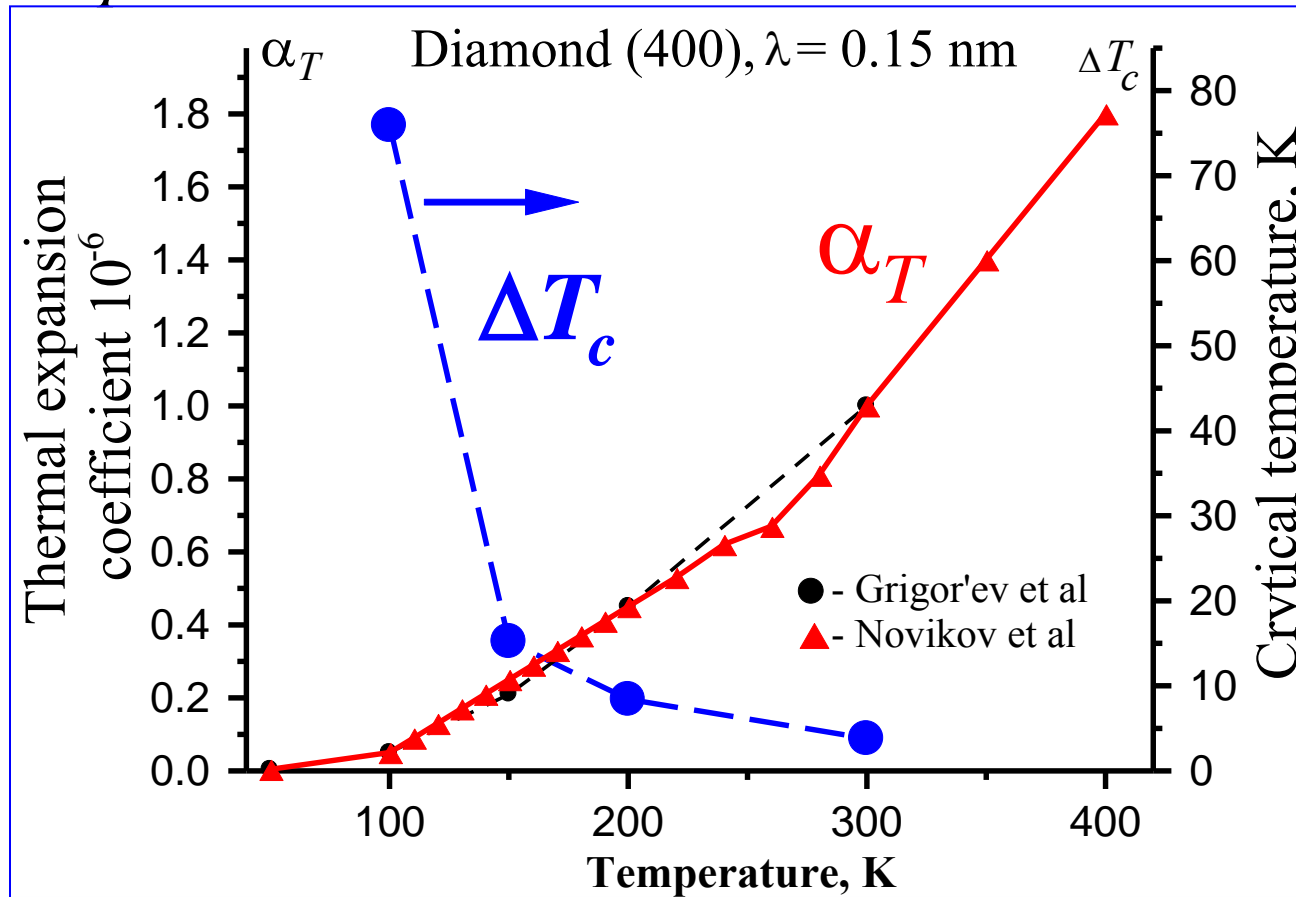
1. Admissible heterogeneity of distribution of temperature in different points of a crystal:

$$\Delta T_c = \Delta \theta_B \operatorname{ctg} \theta_B / 2 \alpha_T,$$



$$\Delta T_c \sim 1-70 \text{ K}$$

where α_T is **linear thermal expansion coefficient**.

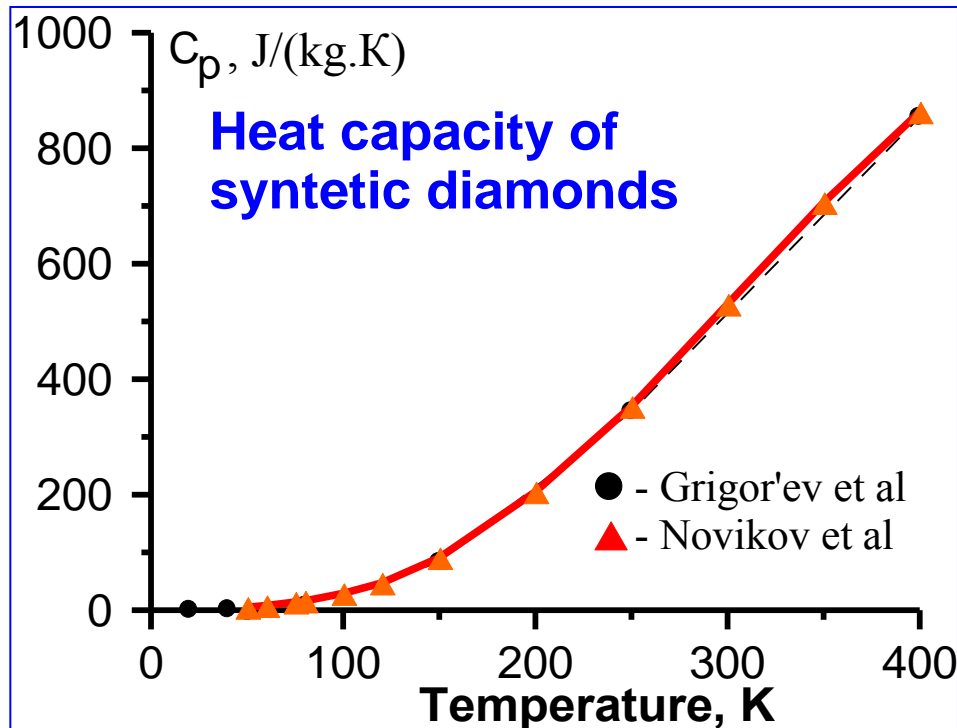


2. Estimation of heat temperature by single pulse:

$$\Delta T_1 = \mu Q_0 / (\pi c \rho r_1^2). \rightarrow \Delta T_1 \sim 0.05\text{-}20 \text{ K}$$

$\lambda_0 = 0.1 \text{ nm}$, $N = 2.8 \cdot 10^{11}$, $Q_0 = 556 \text{ }\mu\text{J}$, absorption part $\eta = \mu l / \gamma_0 \ll 1$,
 $\mu = 3.15 \text{ cm}^{-1}$, $l = 50 \text{ }\mu\text{m}$, Bragg geometry, C(400), $\eta = 0.03$,
 $Q = \eta Q_0 = 15.57 \text{ }\mu\text{J}$, $\rho = 3.52 \text{ g/cm}^3$, $z = 500 \text{ m}$, $r_{1w} = 597 \text{ }\mu\text{m}$,
 $c = (\text{specific heat capacity}) = 510 \text{ J/(kg}\cdot\text{K)}$ at 300 K,

$$\Delta T_1 \approx 0.24 \text{ K}, \rightarrow T_1 = 0.24 \text{ K} \times 2700 = 650 \text{ K} \text{ !!!}$$



3. Characteristic cooling time (heat exchange)

where κ is heat conductivity

$$\tau_T = r_1^2 c \rho / 4 \kappa,$$

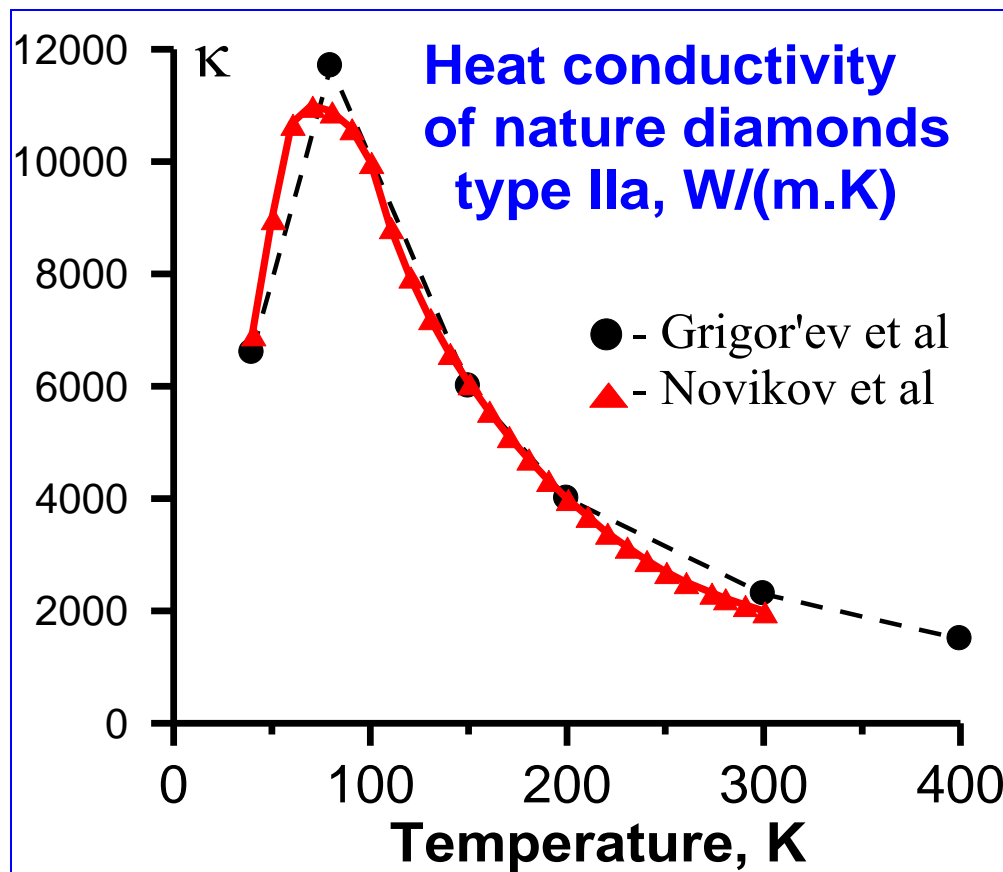
$$(\kappa_{\text{diamond}} / \kappa_{\text{Cu}} \sim 14 - 4) !!$$

Typical values for diamond

$$\tau_T \sim 1\text{-}700 \mu\text{s}$$

Distances between pulses
in the packs $\Delta t_0 = 0.2 \mu\text{s}$

However this time τ_T is much
less than interval of time
between packs 0.1 c
($z > 100 \text{ m}$).



Result such:

Thermal parameters - linear expansion, a thermal capacity and heat conductivity behave in the "opposite" image

(an example – a short blanket).....

Nevertheless, small times of heat exchange τ_T and great values of critical temperature ΔT_c at low temperatures testify to necessity of use of low initial temperature

Thermal conductivity equation

$$c_p \rho (\partial T / \partial t) = \operatorname{div}(\kappa \cdot \operatorname{grad} T) - s(T - T_s) + F,$$

where κ - **heat conductivity**, s – coefficient of heat exchange,
 $F(x, y, z, t)$ – **the density of the heat sources**.

$$F(x, y, t) = \frac{\mu Q_p}{\pi r_1^2} g(x) g(y) f(t)$$

$$g(x) = \exp\left(-\frac{x^2}{r_x^2}\right) \quad g(y) = \exp\left(-\frac{y^2}{r_y^2}\right)$$

$$f(t) = (1 / \pi^{1/2} \tau_0) \sum_{j=1}^p \exp[-(t - t_j)^2 / \tau_0^2]$$

$$T(x, y, t) = \Delta T_1 \sum_{j=1}^p \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} Q_{mn}(t - t_j) S_{mn}(x, y)$$

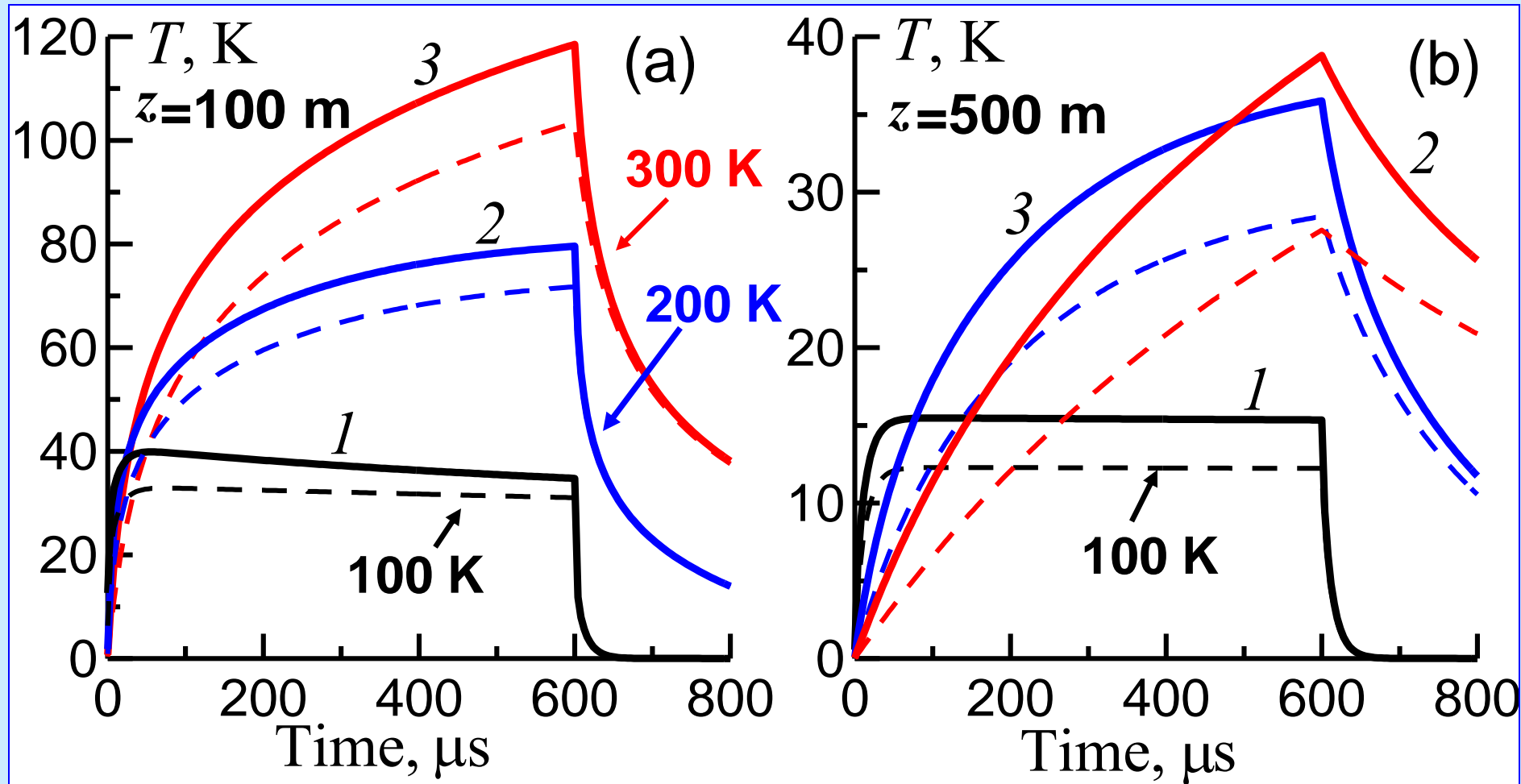
$$Q_{mn}(t - t_j) = \exp[-\underline{a^2}(q_m^2 + q_n^2)(t - t_j)]$$

$$S_{mn}(x, y) = g_{xm} g_{yn} \cos(q_m x) \cos(q_n y)$$

$$g_{im} = (2/L) \int_{-L/2}^{L/2} g_i(\xi) \cos(q_m \xi) d\xi$$

Initial and boundary conditions: $T(x, y, 0) = T_0$, $T(\pm L/2, \pm L/2, 0) = T_0$.

Here $\Delta T_1 = \mu Q_p / (\pi c_p \rho r_1^2)$ – heat temperature at point $x, y = 0$ under the effect of one pulse, **$a^2 = \kappa / c_p \rho$ is the thermal conductivity coefficient**, $q_k = \pi(2k - 1)/L$, $k = m, n$; $i = x, y$.



Dependence of temperature of a crystal on time in a maximum of the pulse ($x=y=0$, *solid curves*) and on its edge ($x=0, y=0.5 r_p$, *dashed curves*) at $z_1 = 100 \text{ m}$ (a) and $z = 500 \text{ m}$ (b) and initial temperatures $T_0 = 100$ (1), 200 (2) и 300 K (3); $Q_p = 80 \mu\text{J}$.

Effect of temperature $T(x, y, t)$ on intensity of reflected and transmitted pulses

The condition of “strong” diffraction: $|\alpha| \leq 2|\chi_h|$

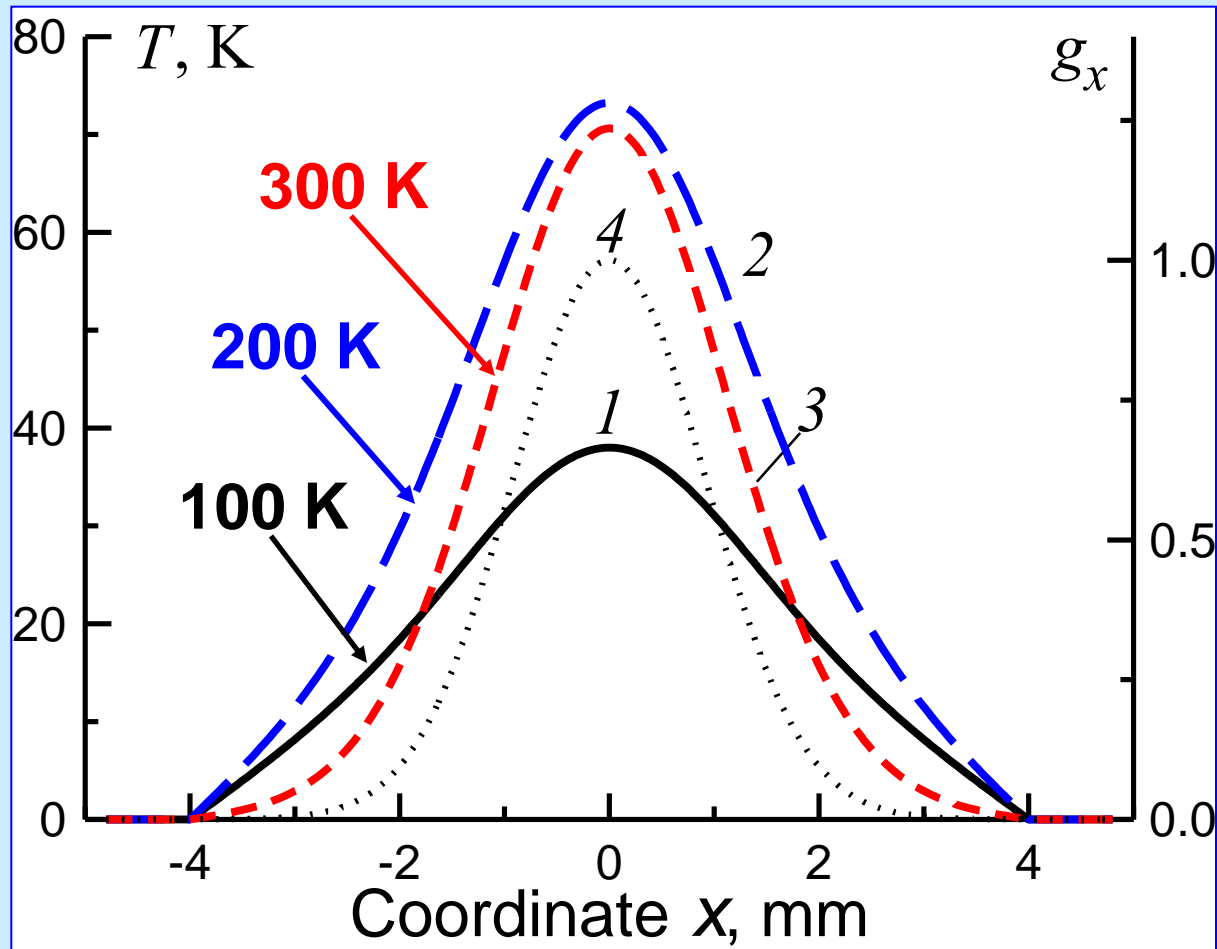
$$\alpha = [k^2 - (\vec{k} + \vec{h})^2] / k^2$$

$$\begin{aligned} \alpha(\Delta\theta, \Omega, T(x, y), q_x) = \\ = 2 \sin 2\theta_B [\Delta\theta + (\Omega / \omega_0 + \alpha_T T) \operatorname{tg} \theta_B - q_x / k_0] \end{aligned}$$

Equation for the intensity of reflected ($C = R$) and transmitted ($C = T$) pulses:

$$I_C(\mathbf{r}, t) = I_0(\mathbf{r}, t) \int_{-\infty}^{\infty} G(\Omega) |C(\alpha)|^2 d\Omega$$

Space distribution of the temperature $T(x, 0, 600 \text{ } \mu\text{s})$



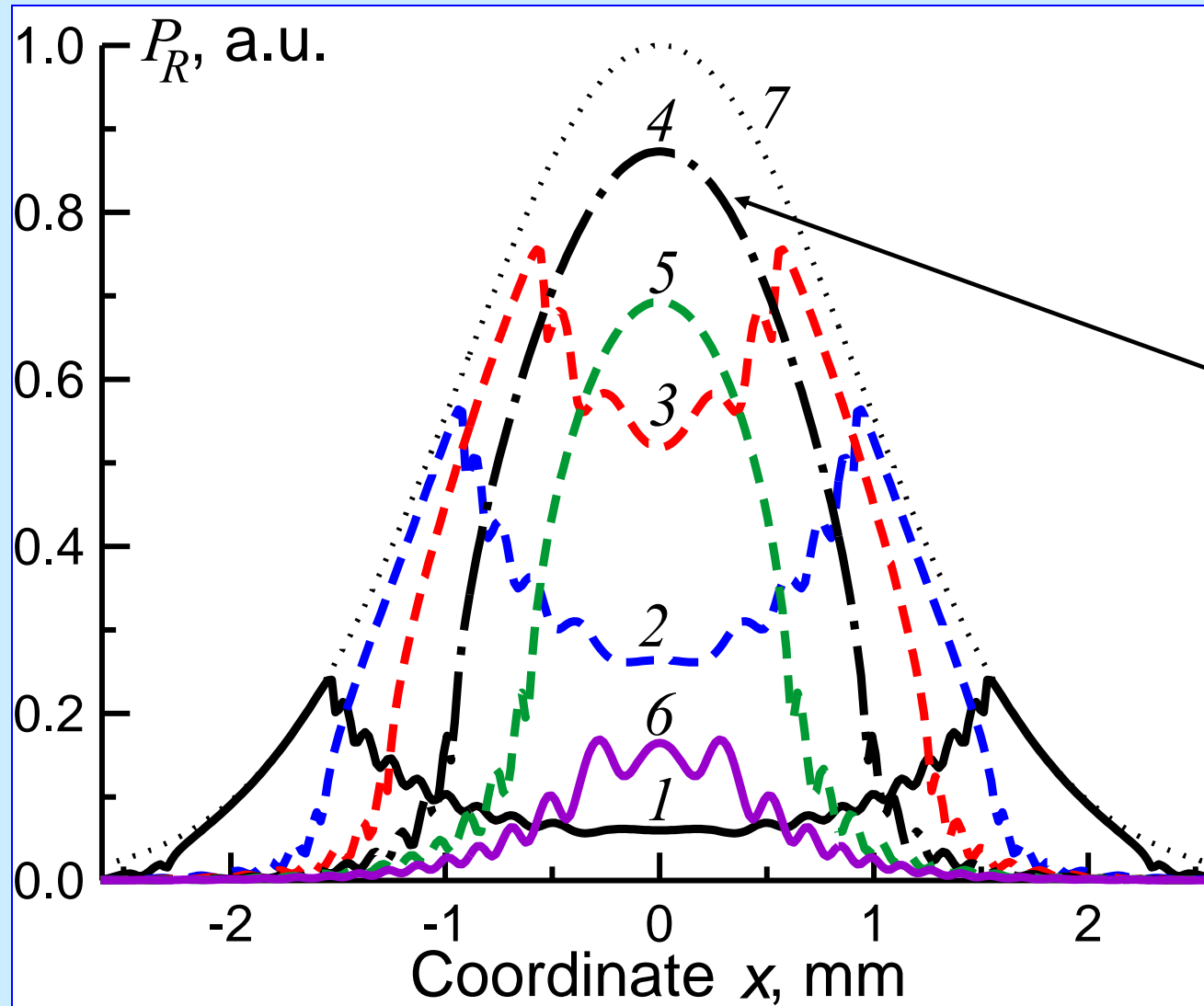
1. At $T_0 = 100 \text{ K}$
 $T_{\text{max}} = 38 \text{ K} < \Delta T_c =$
 $= 75 \text{ K},$

2. At $T_0 = 300 \text{ K}$
It is inverse situation:
 $T_{\text{max}} = 71 \text{ K} \gg \Delta T_c =$
 $= 4 \text{ K}.$

$N = 0.3 \cdot 10^{11} \text{ phot/pulse}$

Space distribution of the temperature $T(x, 0, 600 \text{ } \mu\text{s})$ at initial temperature $T_0 = 100 \text{ K}$ (1), **200 K** (2) и **300 K** (3);
4 – profile of the incident pulse intensity g_x (right scale)

Integral coefficients of reflection $P_R(x)$

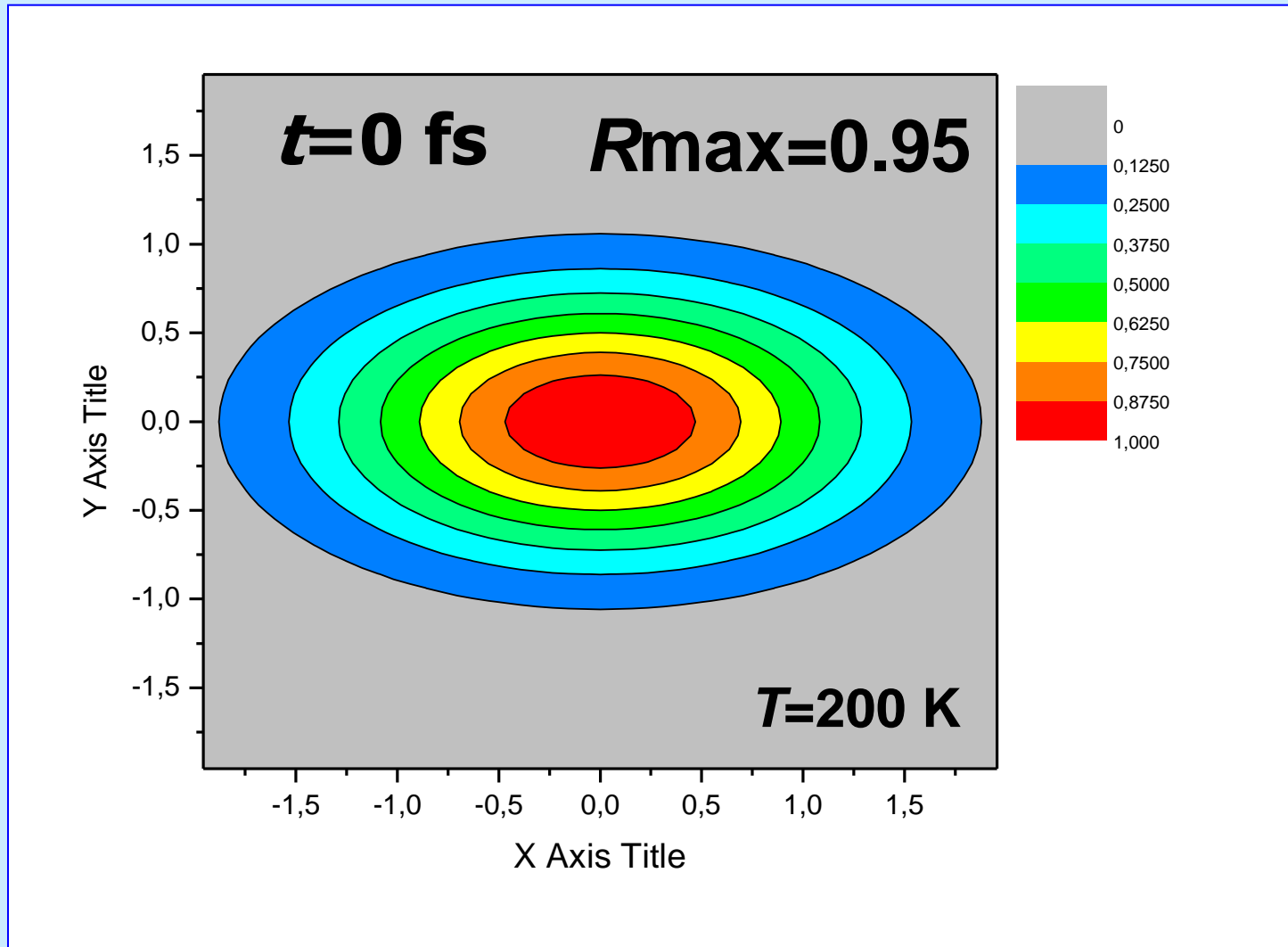


$\varepsilon = \Omega/\Delta\Omega_B$:

- 1 - -2,
- 2 - -3,
- 3 - -3.5,
- 4 - -4,
- 5 - -4.5
- 6 - -5
- 7 - profile $I_0(x)$

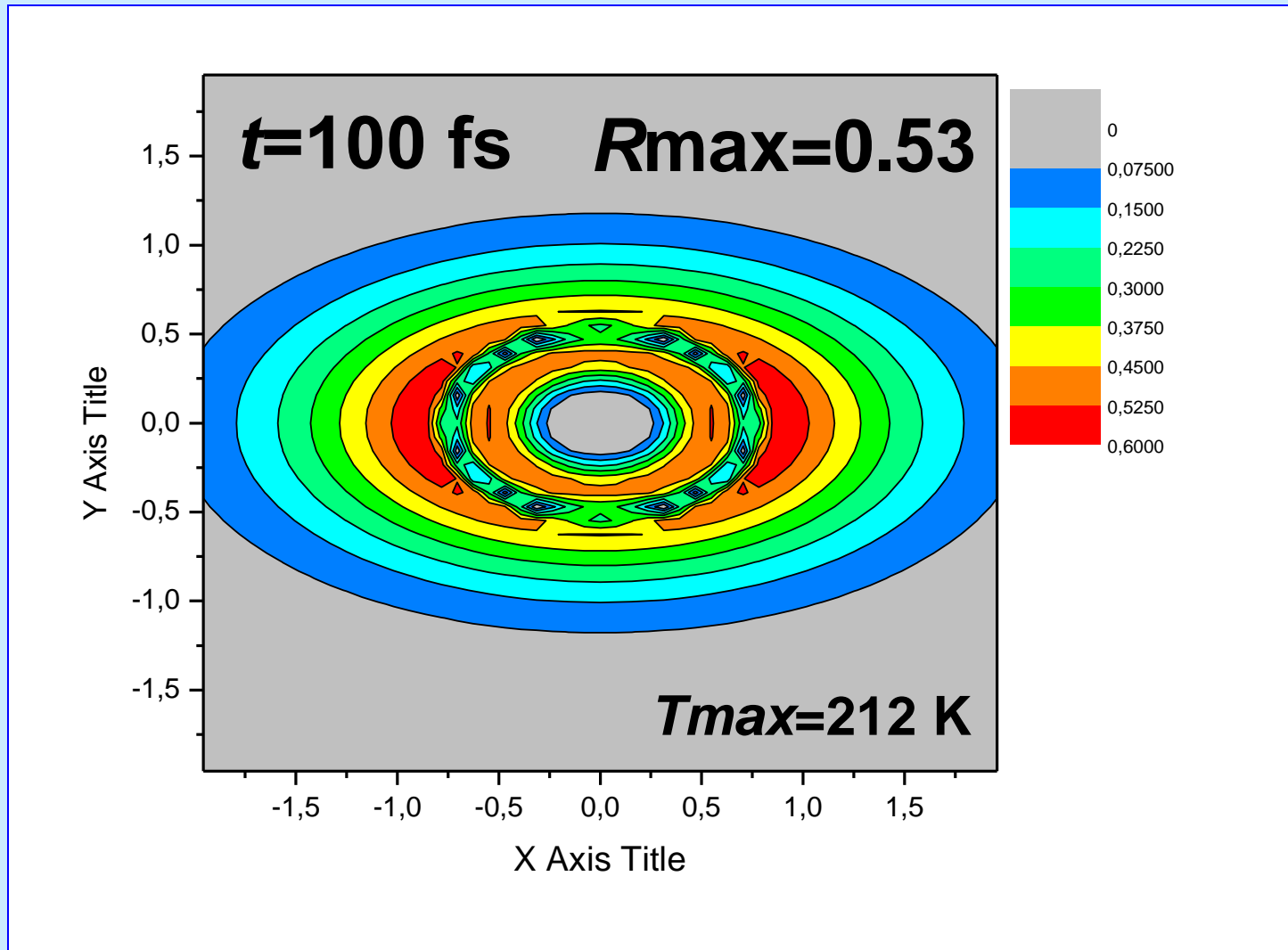
$T_0 = 200 \text{ K},$
 $t = 600 \mu\text{s}$

Map of the intensity distribution of R -pulses $I_R(x, y, t, \Omega = 0)$ during the various moments of time t



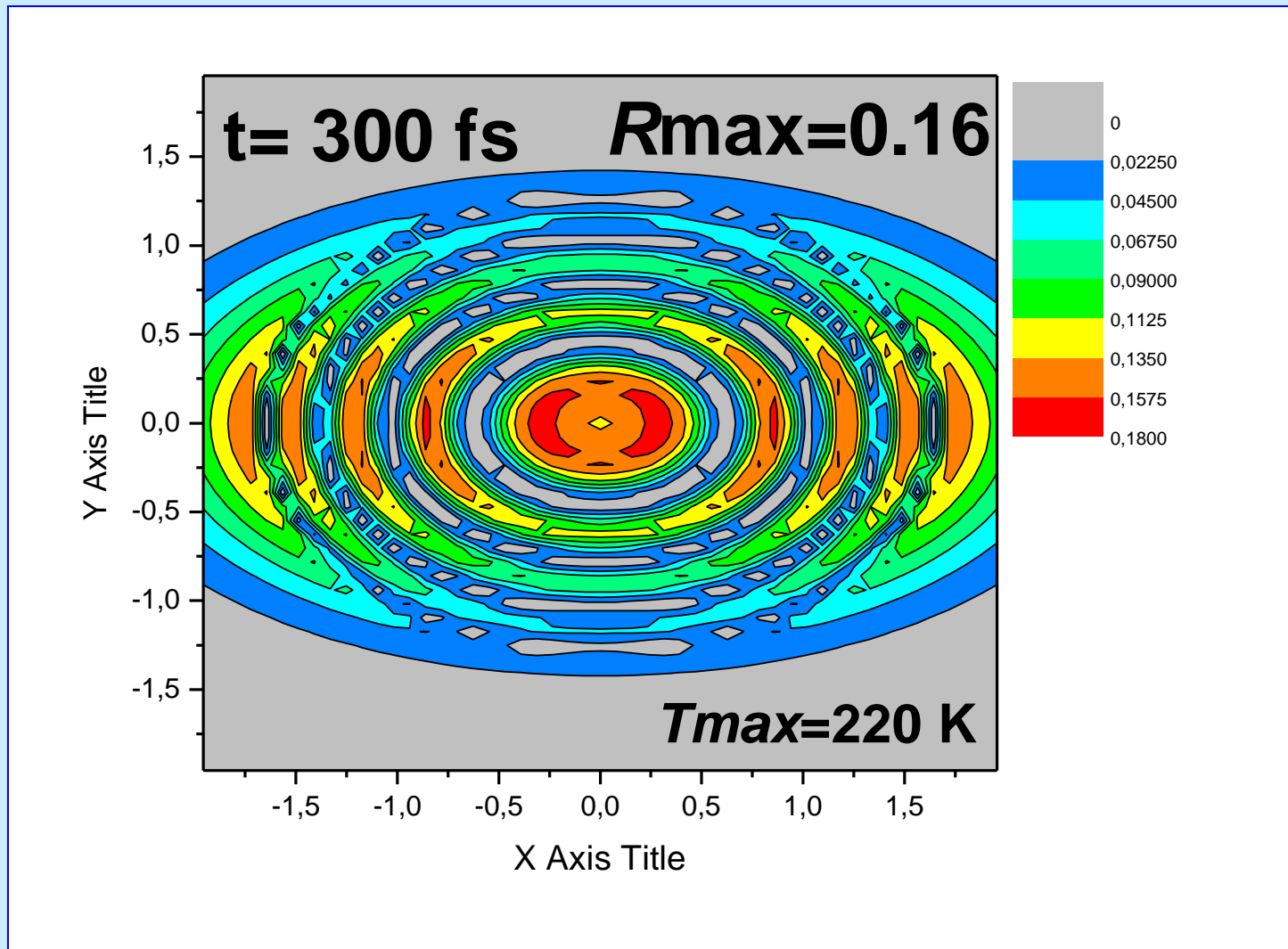
$N = 10^{11}$ photons/pulse, $T = 200$ K, diamond type IIa

Map of the intensity distribution of R -pulses $I_R(x, y, t, \Omega = 0)$ during the various moments of time t



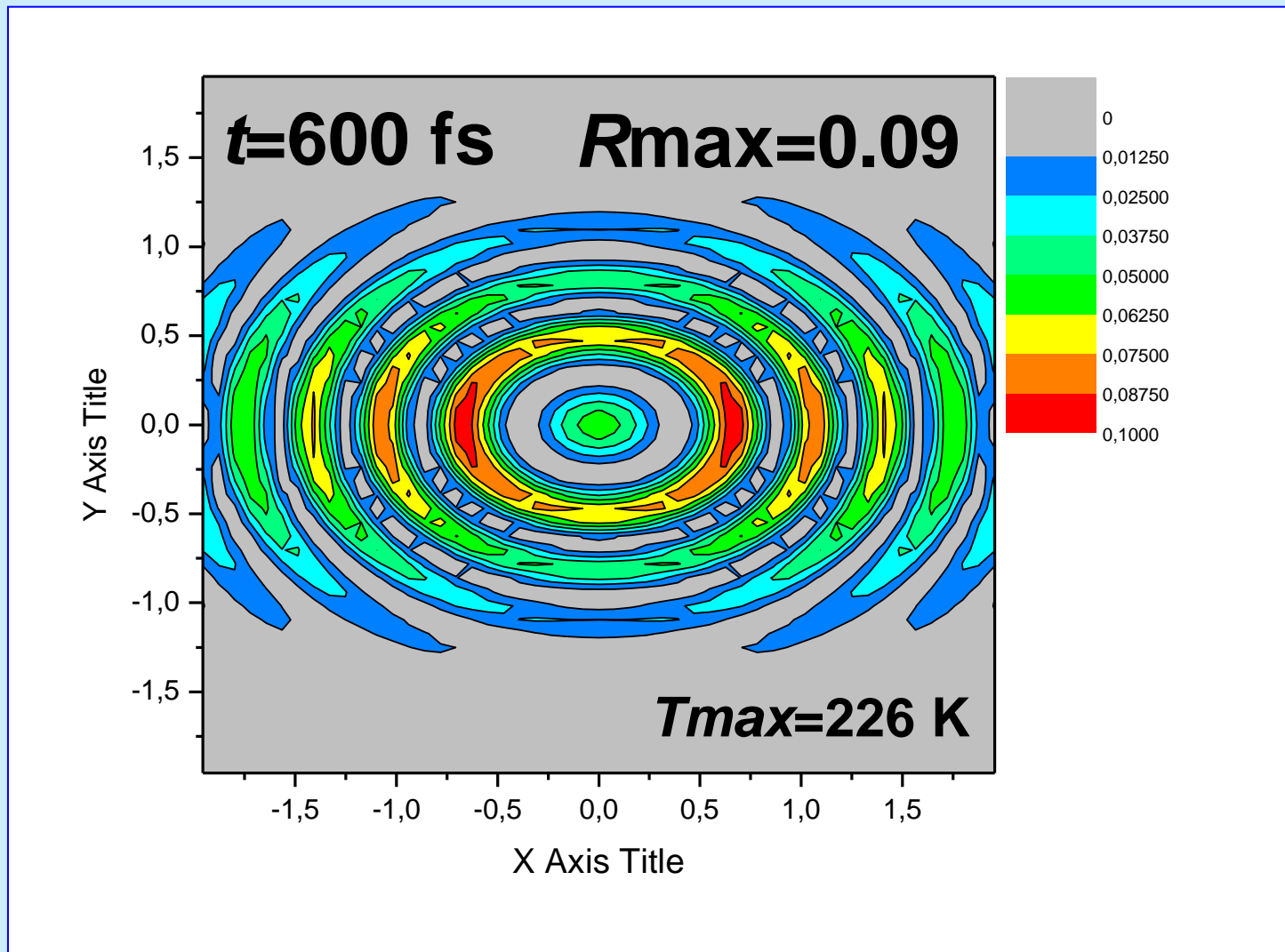
$N = 10^{11}$ photons/pulse, $T = 200$ K, diamond type IIa

Map of the intensity distribution of R -pulses $I_R(x, y, t, \Omega = 0)$ during the various moments of time t



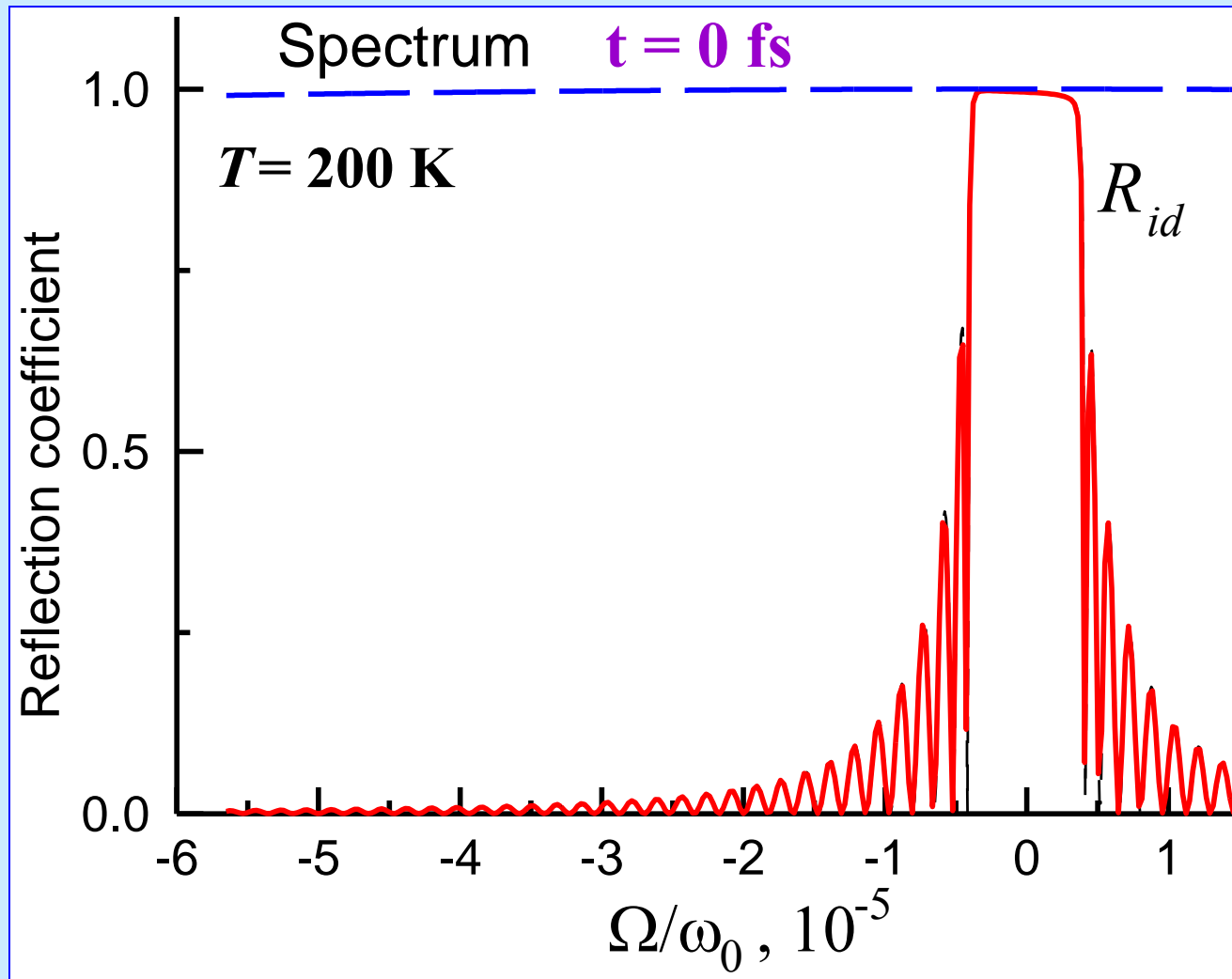
$N = 10^{11}$ photons/pulse, $T = 200$ K, diamond type IIa

Map of the intensity distribution of R -pulses $I_R(x, y, t, \Omega = 0)$ during the various moments of time t



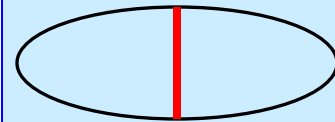
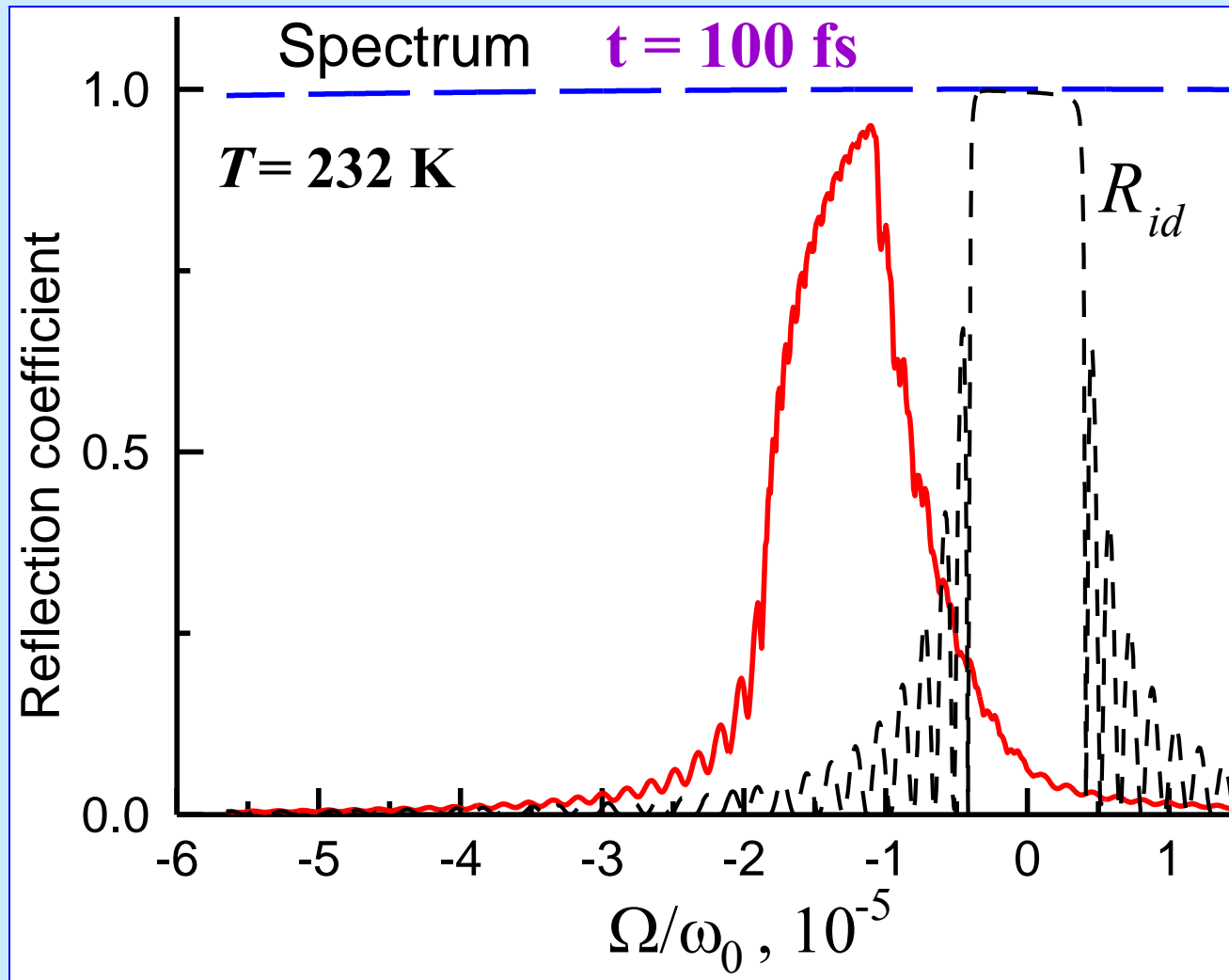
$N = 10^{11}$ photons/pulse, $T = 200$ K, diamond type IIa

Spectral reflection coefficient at different moments of time



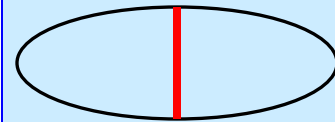
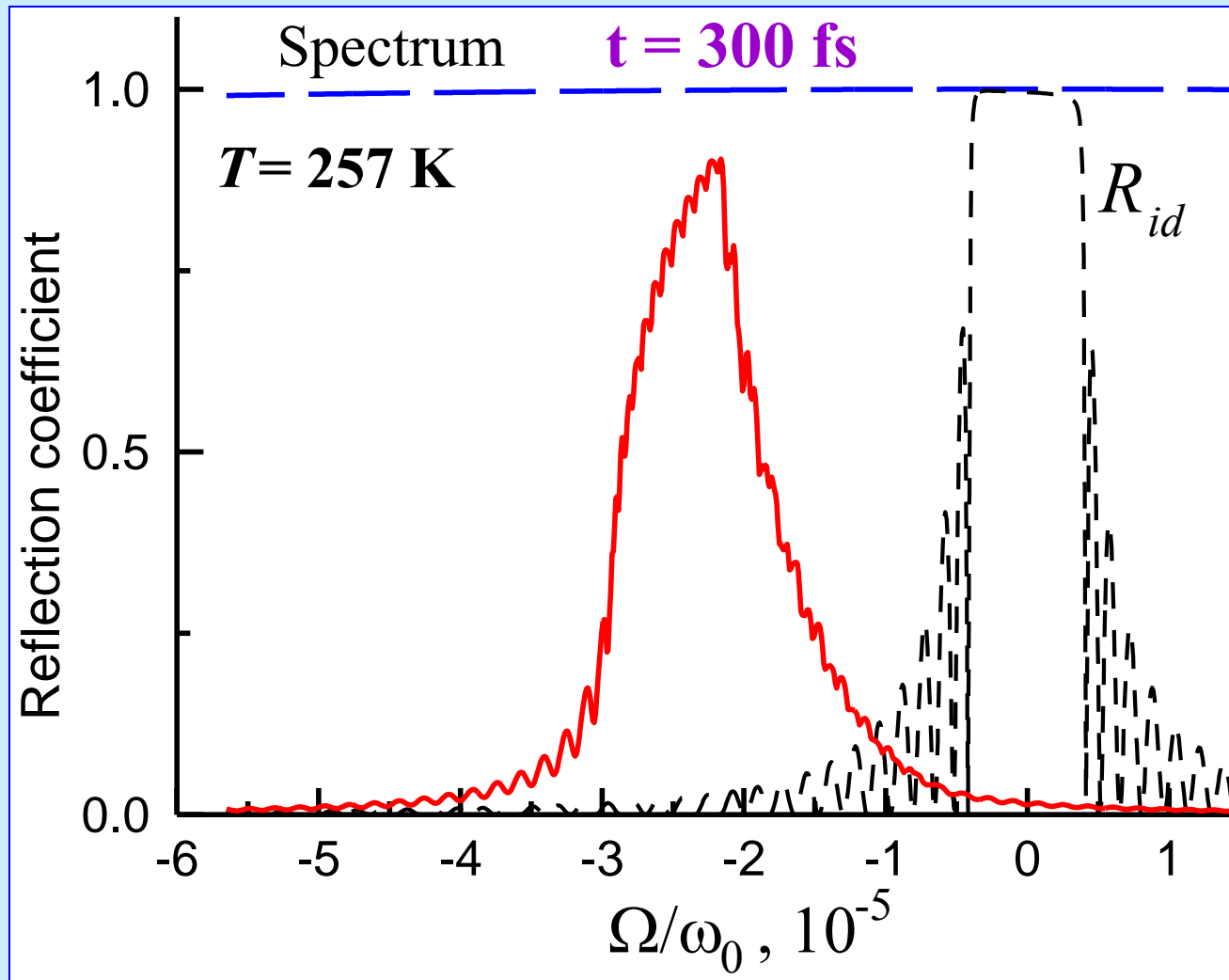
$$N = 2.8 \cdot 10^{11}, T_0 = 200 \text{ K}, \Delta T_c = 8.4 \text{ K}.$$

Spectral reflection coefficient at different moments of time



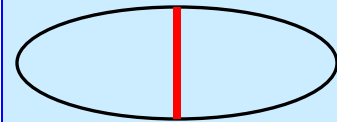
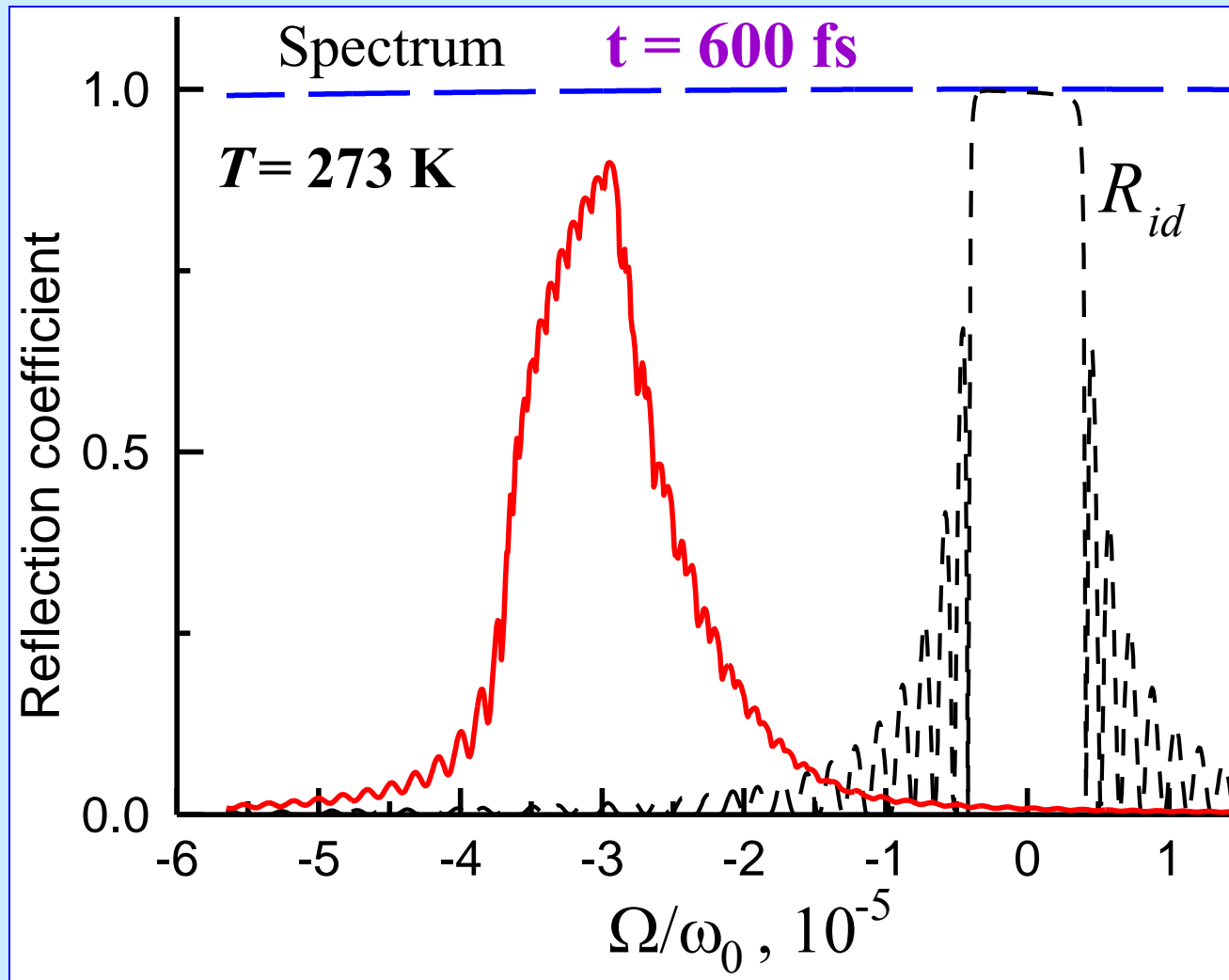
$$N = 2.8 \cdot 10^{11}, T_0 = 200 \text{ K}, \Delta T_c = 8.4 \text{ K.}$$

Spectral reflection coefficient at different moments of time



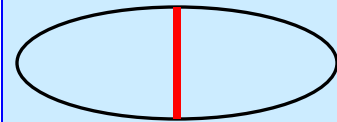
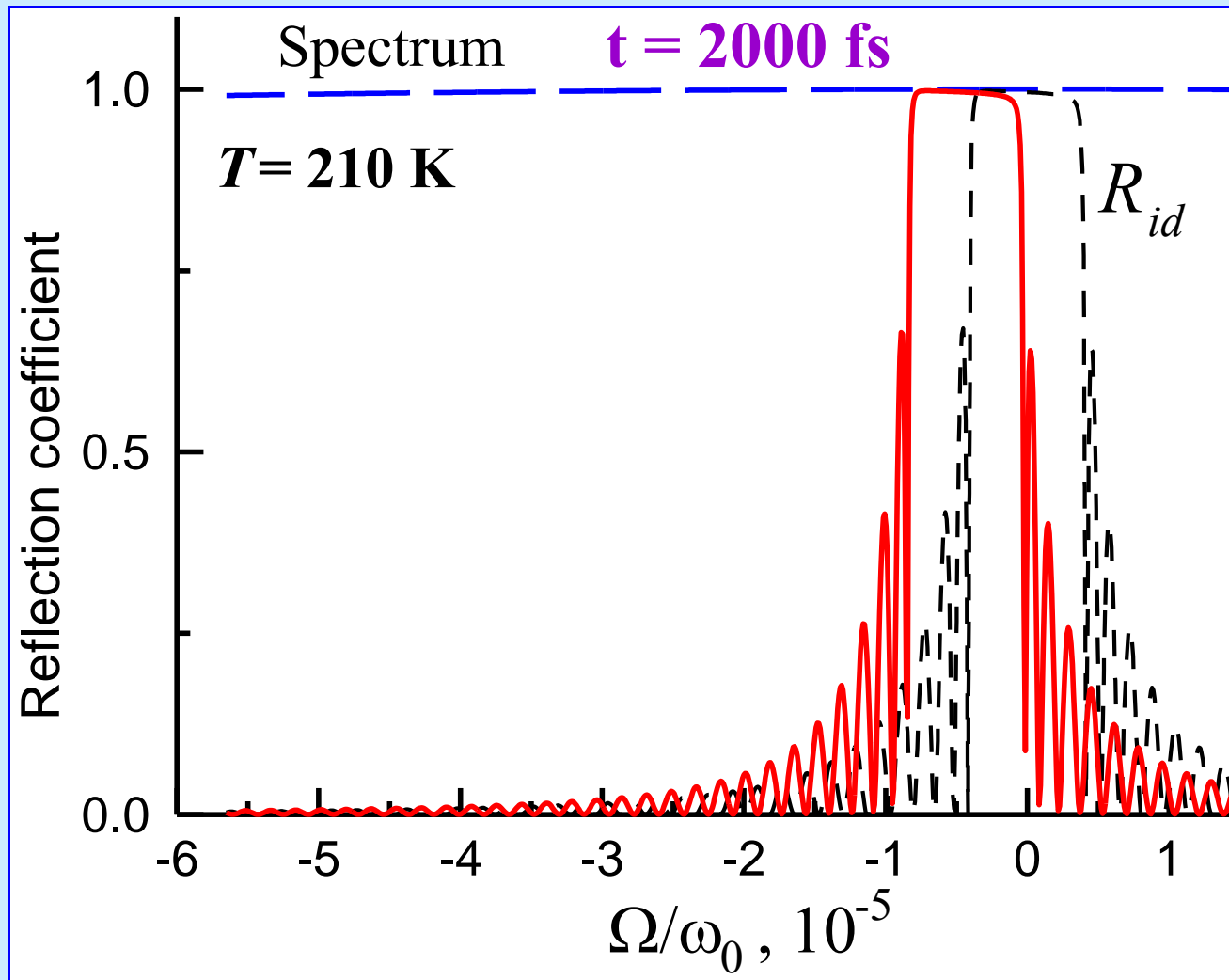
$$N = 2.8 \cdot 10^{11}, T_0 = 200 \text{ K}, \Delta T_c = 8.4 \text{ K}.$$

Spectral reflection coefficient at different moments of time

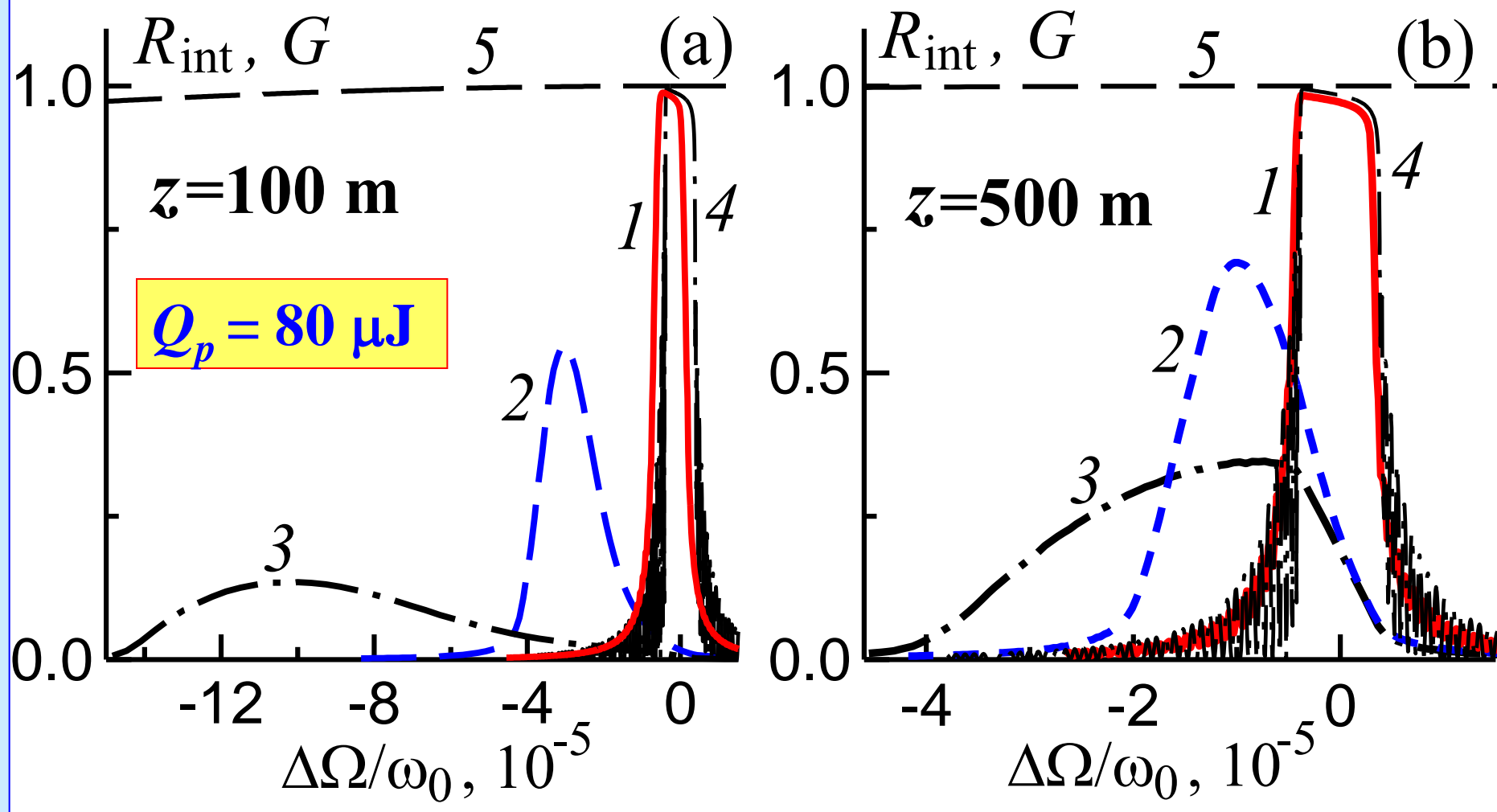


$$N = 2.8 \cdot 10^{11}, T_0 = 200 \text{ K}, \Delta T_c = 8.4 \text{ K.}$$

Spectral reflection coefficient at different moments of time

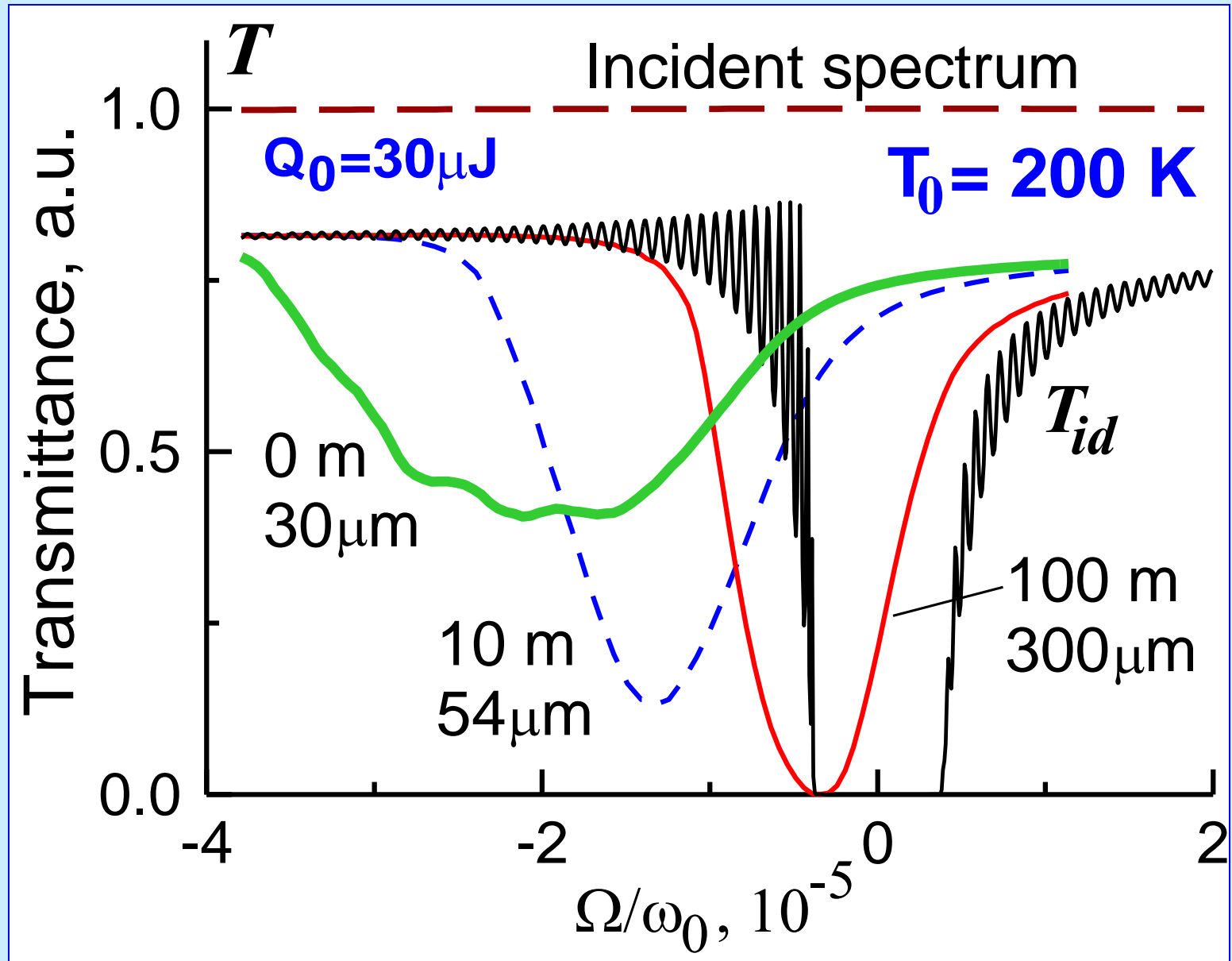


$$N = 2.8 \cdot 10^{11}, T_0 = 200 \text{ K}, \Delta T_c = 8.4 \text{ K.}$$



Integrated coefficient of reflection R_{int} at initial temperatures $T_0 = 100$ (1), 200 (2) and 300 K (3) on the distances $z = 100 \text{ m}$ (a) and $z = 500 \text{ m}$ (b) from XFEL, 4 – reflection coefficient an ideal crystal, 5 – a spectrum of the incident pulses with a width $\Delta\Omega_c = 2/\tau_c$, where $\tau_c \approx 0.2 \text{ fs}$ is the time of coherence.

Integral spectral coefficient of transmission



Conclusions:

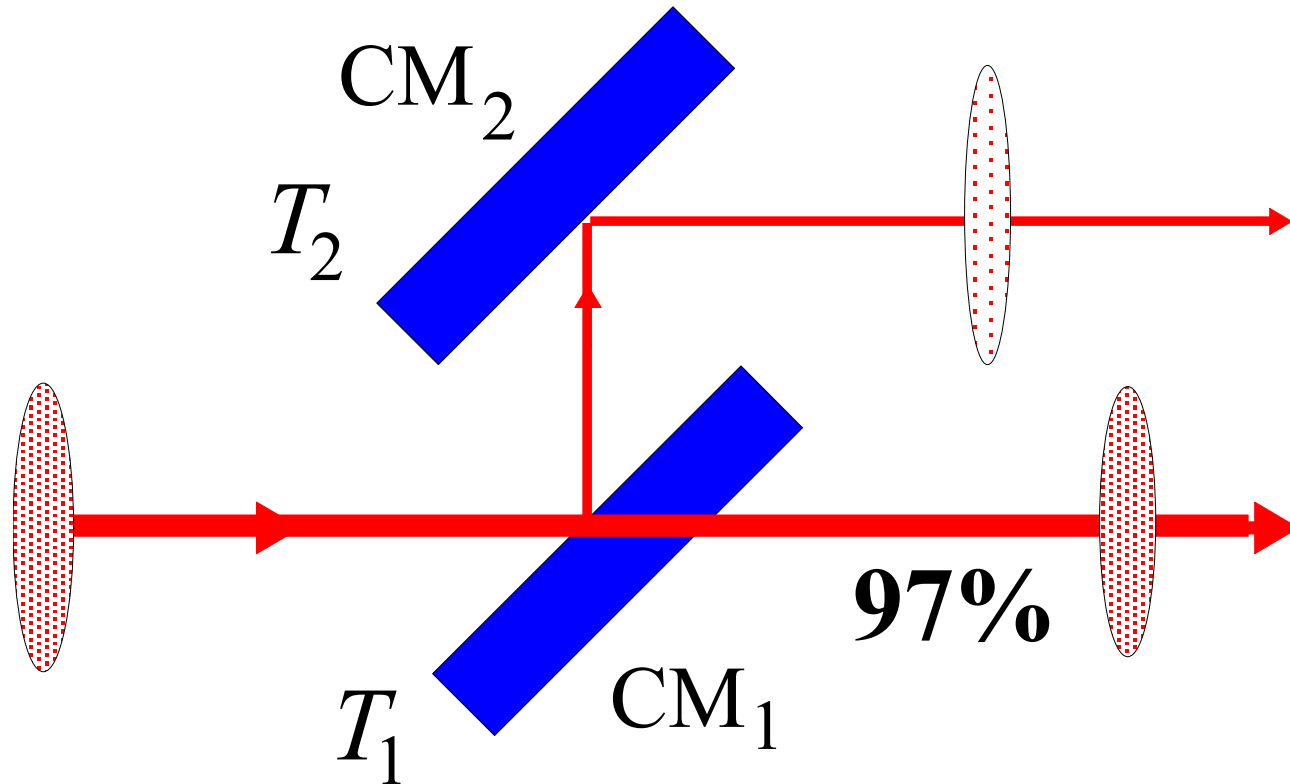
1. Within the limits of two-dimensional thermal conductivity equation with the distributed sources spatiotemporal distributions of the crystal temperature $T(x, y, t)$ under action of XFEL pulses are calculated.
2. In the case of pulses with great and middle intensity the temperature of a crystal heating reach up to 100-300 K. However, the main problem is the big gradient of temperature exceeding critical values $T_c \sim 1-10$ K.
3. For pulses **of low power** ($N \sim 10^{10}$ photons/pulse conditions of diffraction are carried out at the distances of order 800 meters.
4. It is desirable "to work" at initial temperature $T_0 \sim 100-200$ K with optimal speed of heat removal.
5. It is necessary consideration of a problem taking into account temperature and time dependence of all thermal-physical parameters.

Acknowledgments

- 1. The Russian Foundation for Basic Research, Projects № 10-02-00768, 12-02-00924;**
- 2. The German Federal Ministry of Education and Research (BMBF), project no. 05K10CHG.**

Thanks for your attention

Проблема: $T_1(x, t) > T_2 \approx \text{const}$



Схематическое изображение кристаллов CM_1 и CM_2 в схеме двухкристального рентгеновского монохроматора. Очевидно, что температура $T_1(x, t) > T_2 \approx \text{const}$.

