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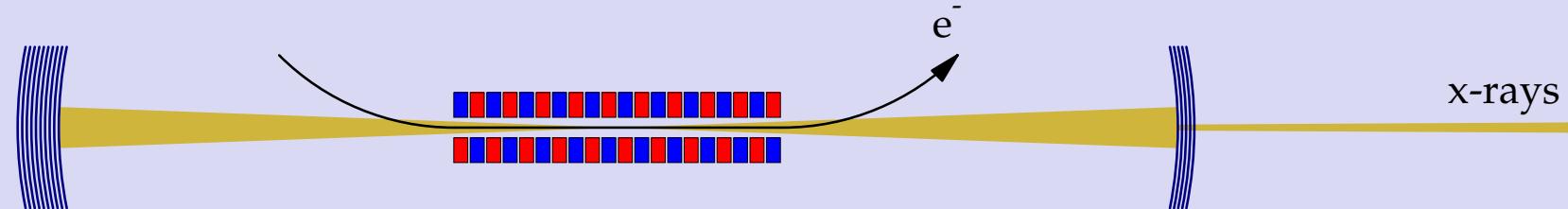


U.S. DEPARTMENT OF ENERGY

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# Feasibility of Diamond Cavities for X-Ray Free Electron Laser Oscillator

*Yuri Shvyd'ko*



**In collaboration with**

*K.-J. Kim, R. Lindberg, S. Stoupin, H. Sinn, A. Cunsolo*

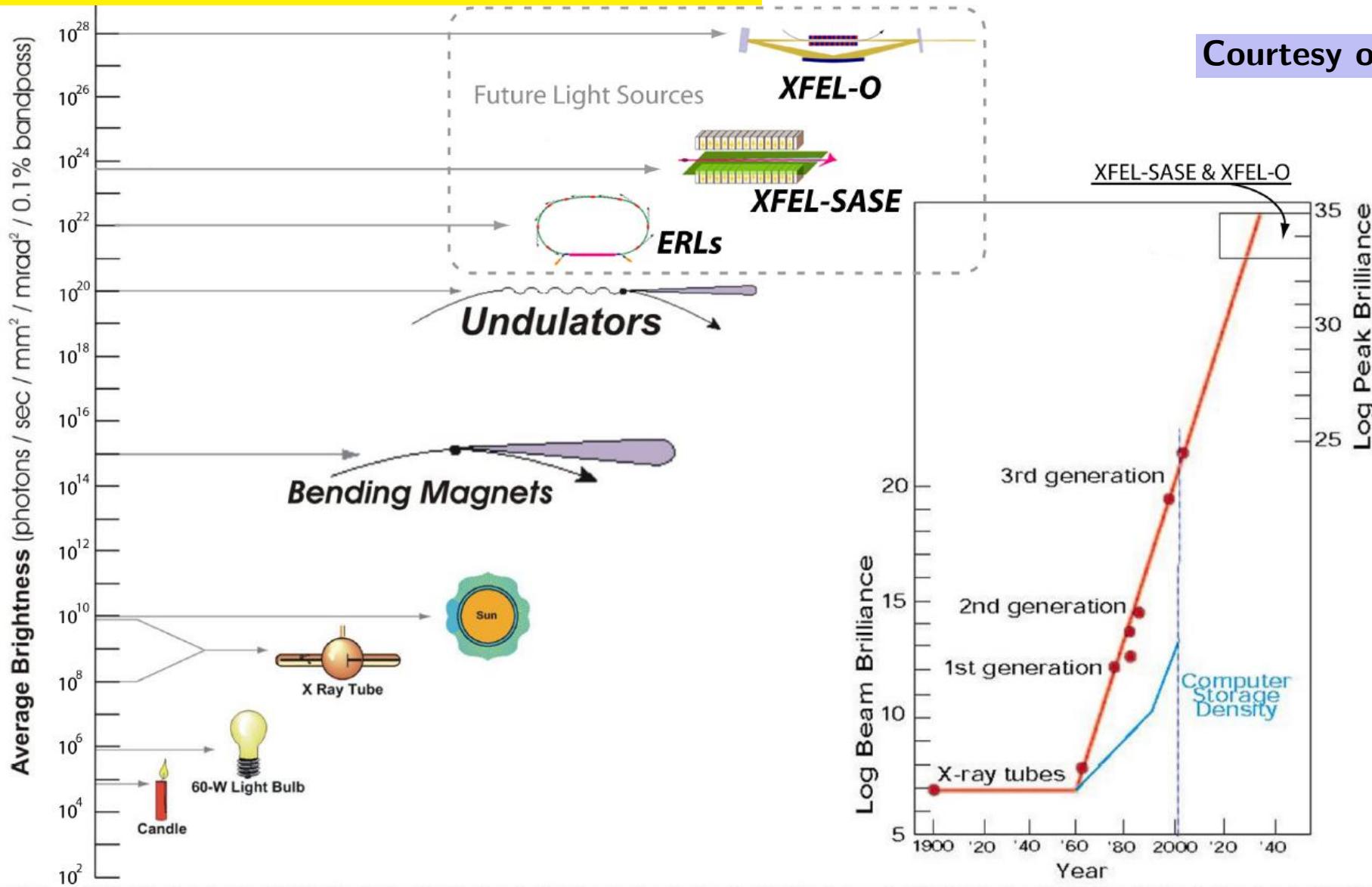
# Content

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- **Coherent x-ray sources**
- **XFEL-O concept**
- **X-ray cavities**
- **Feasibility of the diamond cavities - first experiments:**
  - Spectral bandwidth and reflectivity
  - Low temperature thermal expansion
  - Heat load simulation
  - Nanoradian stability
- **Conclusions, and Outlook.**

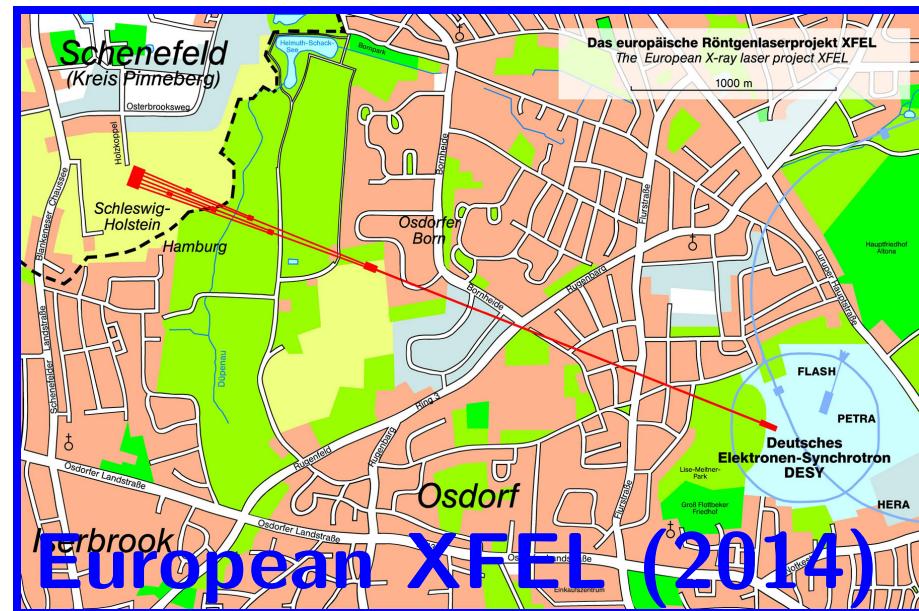
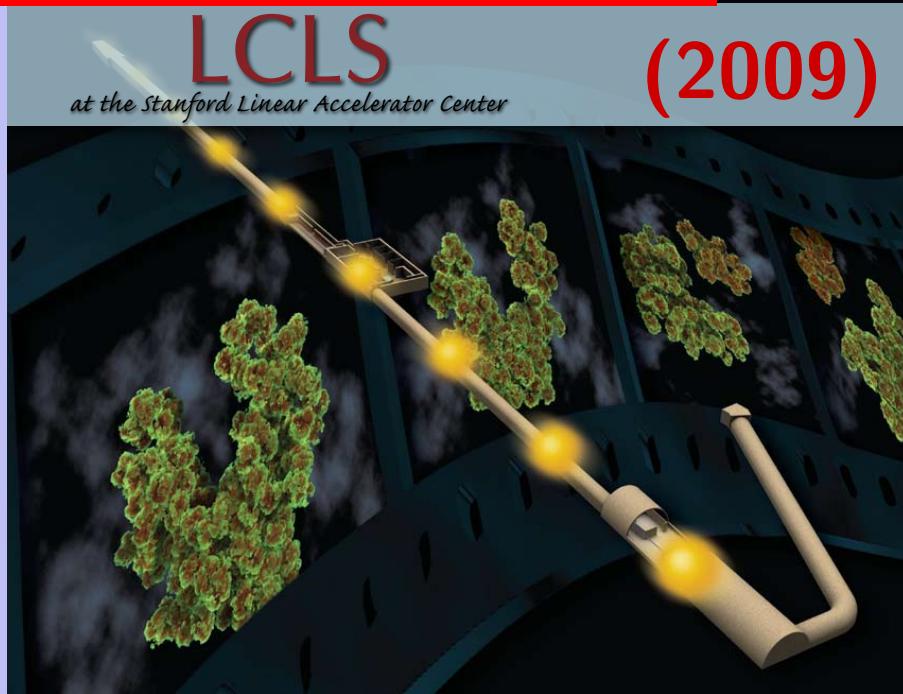
# Present and Future X-Ray Sources

## Future: linac-based x-ray sources



Courtesy of K.-J. Kim

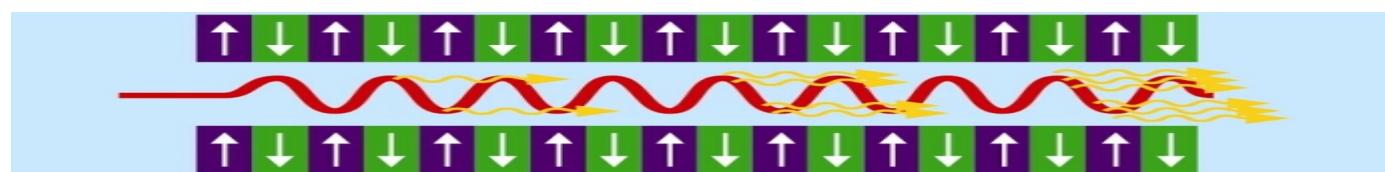
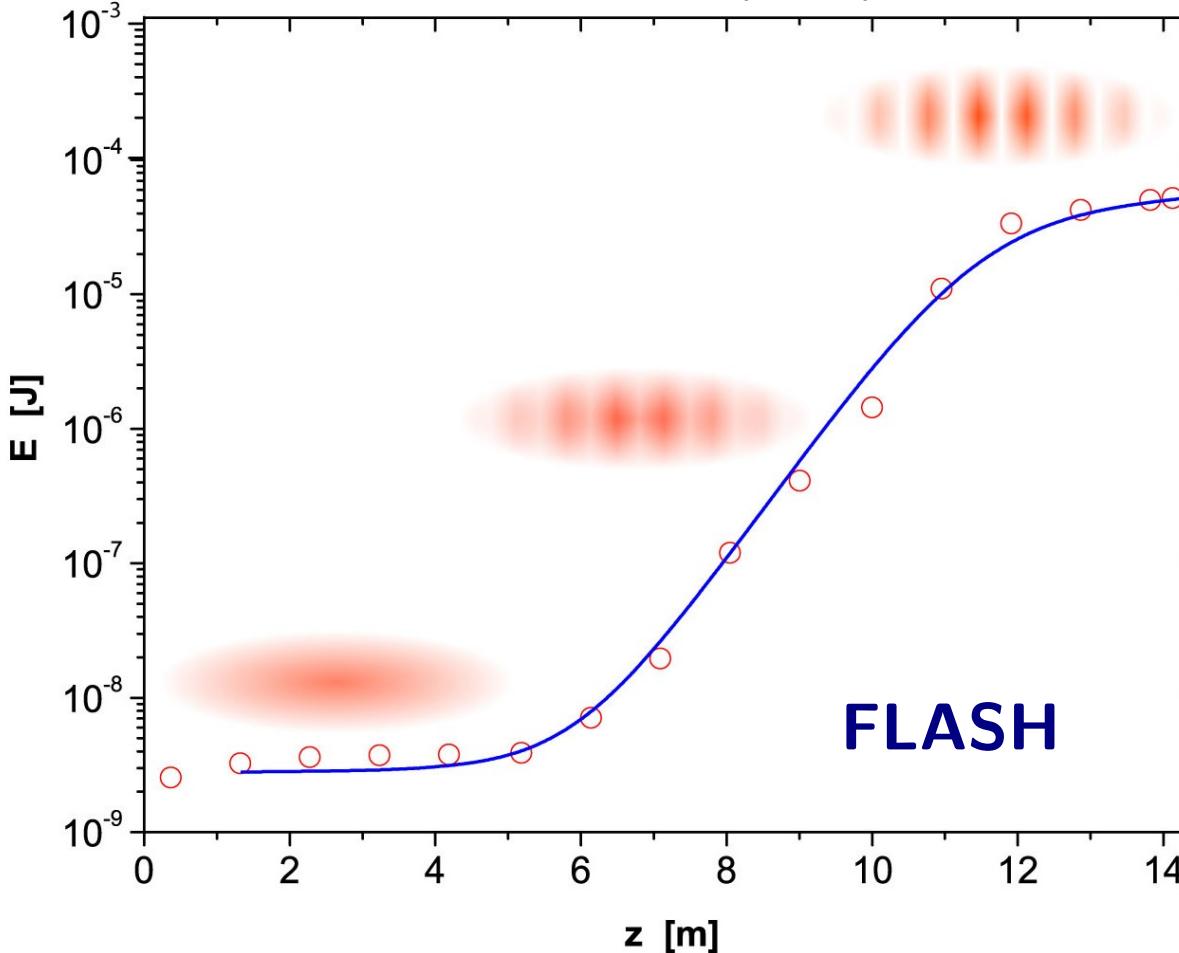
# HG-XFEL Facilities



# High-Gain SASE XFEL by Microbunching

Kondratenko, Saldin (1979)

Bonifacio, Pellegrini, Narducii (1984)



⇒ In the beginning without microbunching all the  $N$  electrons can be treated as individually radiating charges, and the resulting spontaneous emission power is proportional to  $N$ .

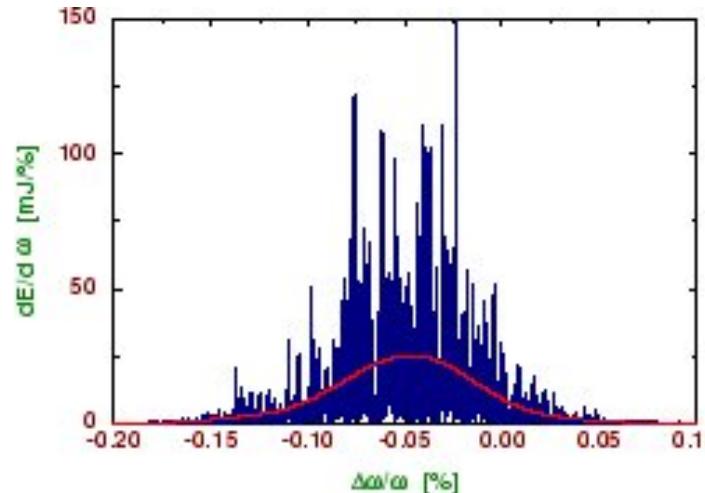
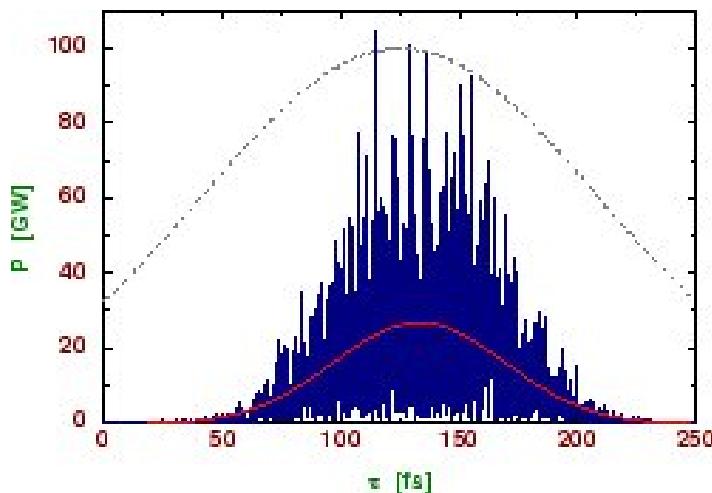
⇒ The shot noise of the electron beam is amplified up to complete microbunching.

⇒ With complete micro-bunching, all electrons radiate almost in phase. This leads to a radiation power growth as  $N^2$ , a process called self-amplified spontaneous emission (SASE)

Requires electron beams:  
emittance  $\epsilon_n \lesssim 10^{-6} \text{ m rad}$   
energy  $E_e \simeq 10 \text{ GeV}$   
energy spread  $\frac{\sigma_E}{E_e} \lesssim 10^{-4}$   
peak current  $\simeq 10^4 \text{ A}$   
pulse length  $\lesssim 100 \text{ fs}$

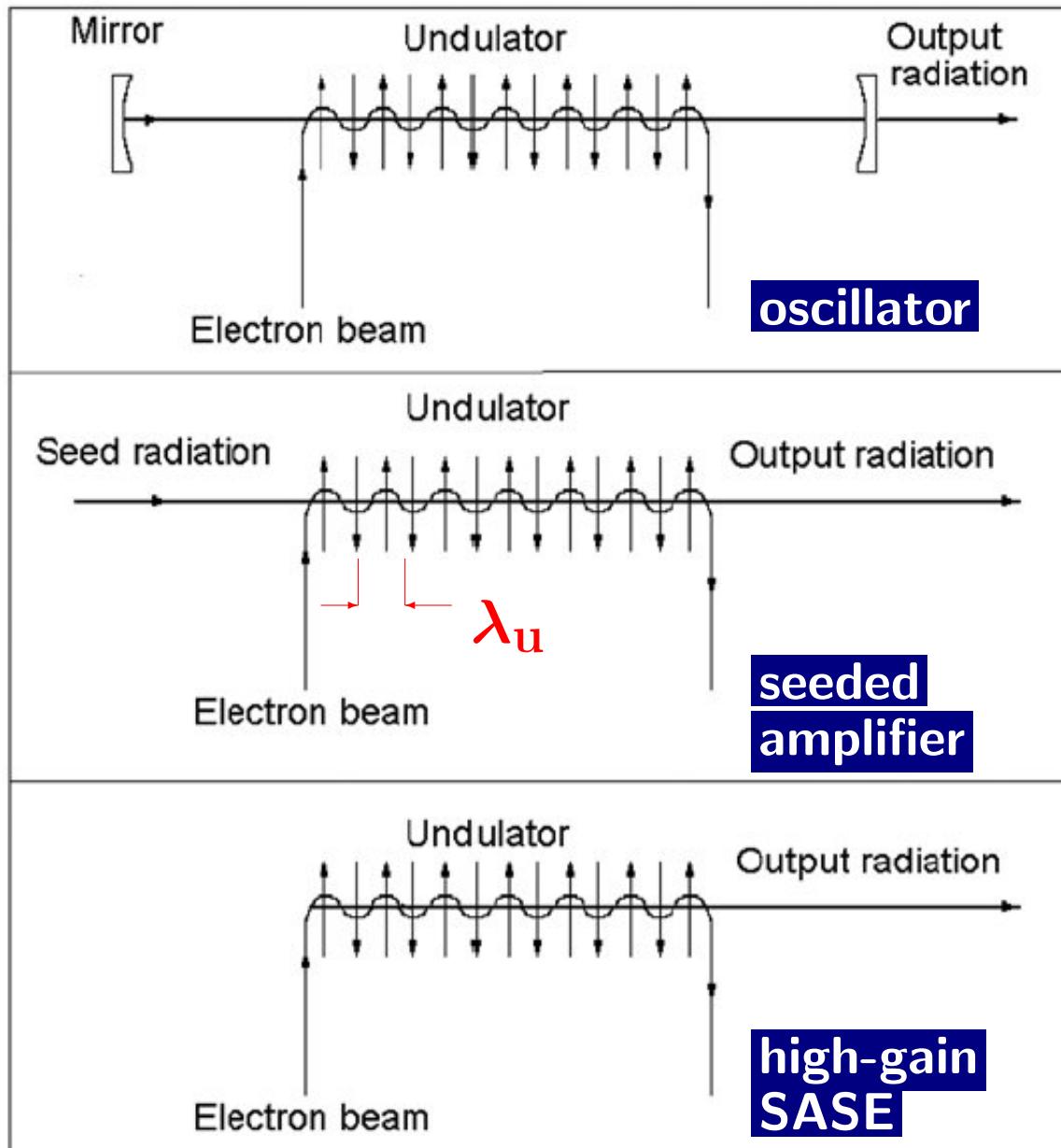
# Coherent Properties of the HG-XFEL Radiation

- The radiation from a SASE XFEL is fully transversely coherent, nearly Fourier transform limited.
- Temporal coherence is low because of the start-up from noise.



- Seeded **FEL amplifier** or **FEL oscillator** would generate radiation with better coherent properties.

# FEL configurations



The essential advantage of FEL radiation as compared to undulator radiation is its much higher intensity because a large number  $N$  of electrons radiate coherently:  $\propto N^2$ , producing a clean superradiant pulse.

Require electron beams:

emittance  $\varepsilon_n \lesssim 10^{-6} \text{ m rad}$

energy  $E_e \simeq 10 \text{ GeV}$

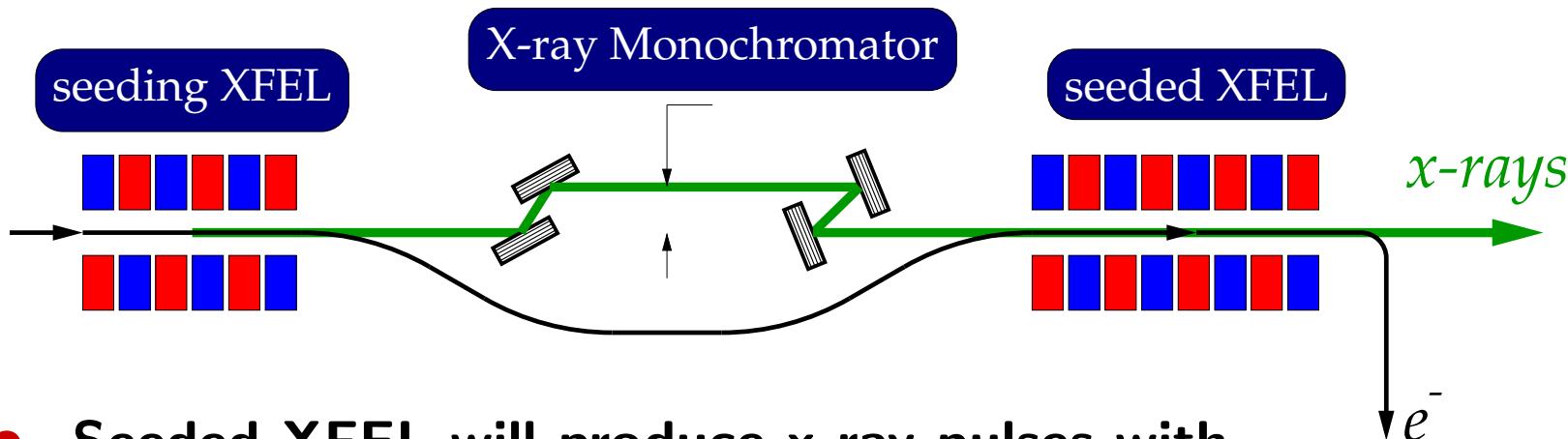
energy spread  $\frac{\sigma_E}{E_e} \lesssim 10^{-4}$

peak current  $10 - 10^4 \text{ A}$

Resonance condition:

$$\lambda = \frac{\lambda_u}{2\gamma^2}(1 + K^2)$$

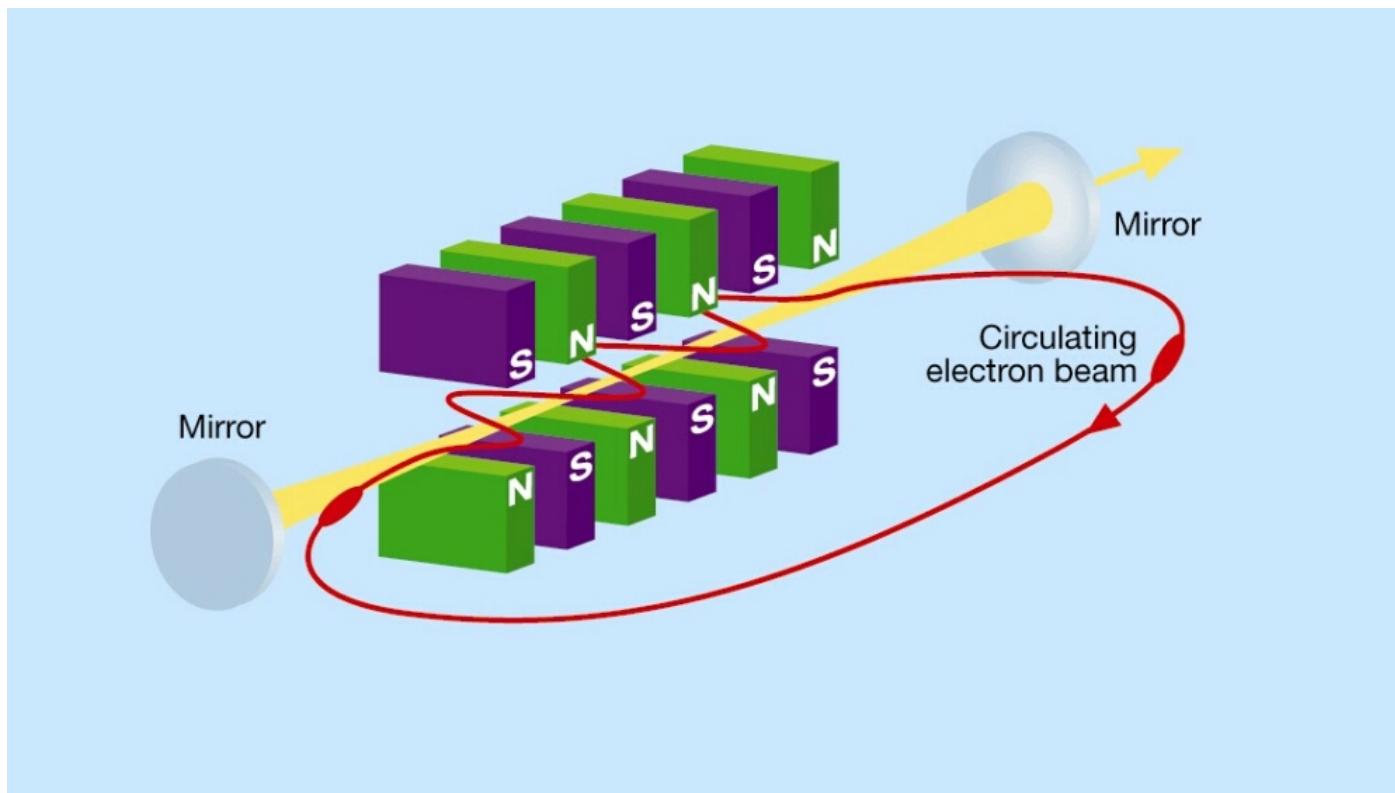
# Seeded (Two-Stage) XFEL



- Seeded XFEL will produce x-ray pulses with
  - $\simeq 9 \times 10^{11}$  photons/pulse ( $2 \text{ mJ/pulse} = 20 \text{ GW}$ )
  - $\simeq 4 \times 10^{16}$  photons/s ( $100 \text{ W}$ )
  - **transversely and temporarily coherent**
  - $\Delta E \approx 20 \text{ meV}$  (rms) close to the limit given by the pulse duration  $\tau_e \approx 0.1 \text{ ps}$  (rms).
- Considered as upgrade of the European XFEL (>2014).
- E.L. Saldin, E.A. Schneidmiller, Yu.V. Shvyd'ko, and M.V. Yurkov, "X-ray FEL with a meV bandwidth", NIM, A475 (2001) 357-362.
- The Technical Design Report of the European XFEL, July 2007

# Is an XFEL-Oscillator Feasible?

First proposal: Colella and Luccio (1984)



FELs based on the oscillator principle are limited, on the short-wavelength side, to ultraviolet wavelengths, primarily because of **mirror limitations**.

Free-electron lasing at wavelengths shorter than ultraviolet **can be achieved with a single-pass, high-gain FEL amplifier only**.

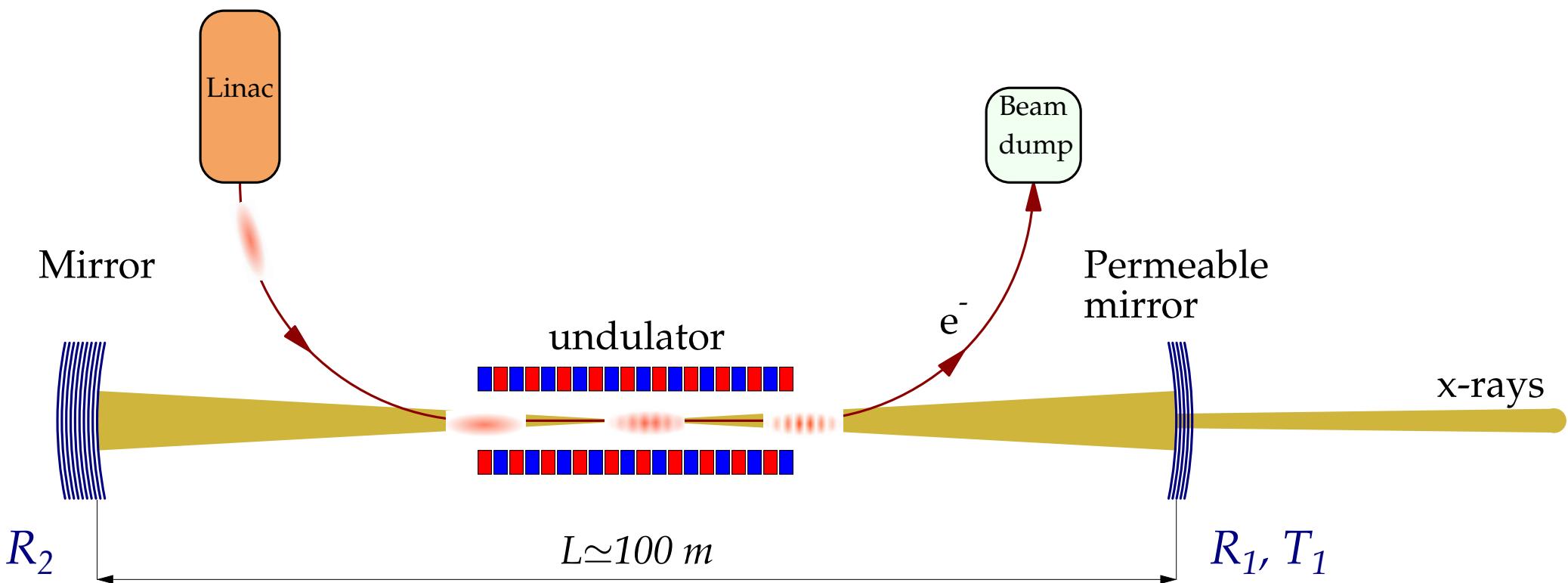
(The Technical Design Report of the European XFEL, July 2007)

# XFEL-Oscillator Feasibility

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- Low-gain XFELO is feasible based on:
    - low-loss x-ray crystal cavity (losses  $\simeq 15\%$ ),
    - ultra-low-emittance ( $\epsilon_n \lesssim 10^{-7}$  m rad) electron beams.
  - K.-J. Kim, Yu. Shvyd'ko, S. Reicher, PRL 100 (2008) 244802.
-

# X-FEL Oscillator Principles

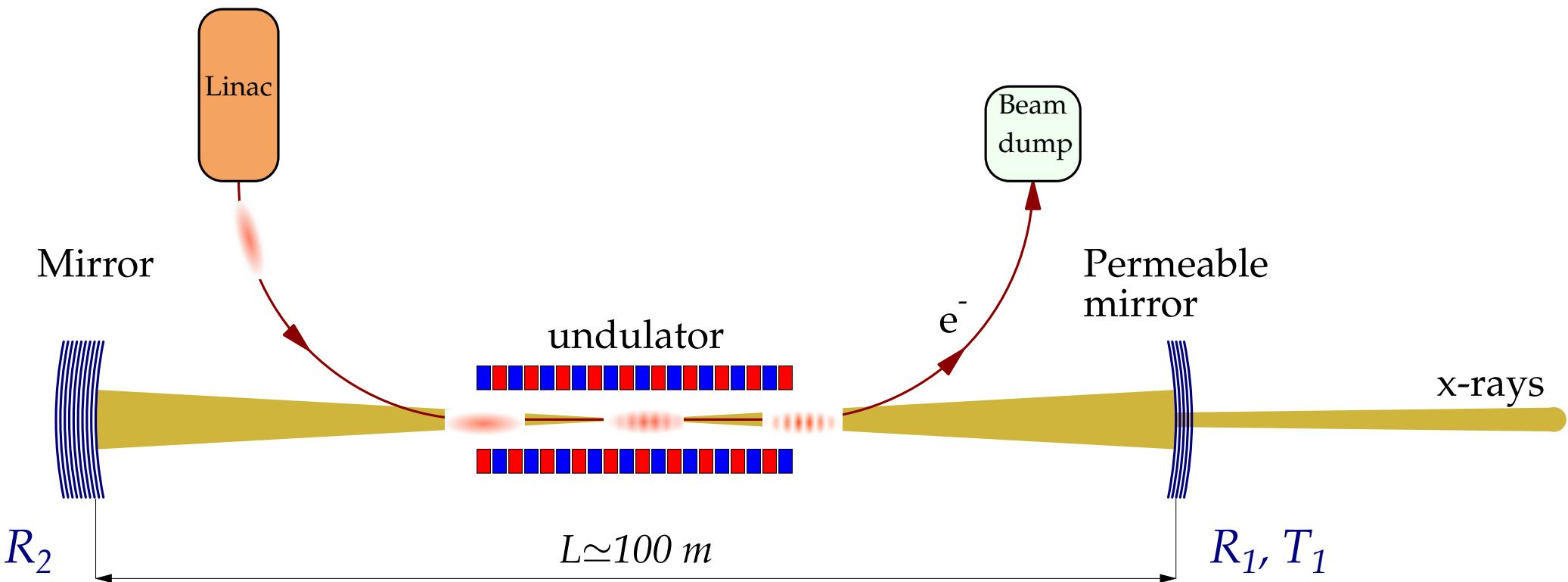


High repetition rate is required:  $\nu = c/2L \simeq 1 \text{ MHz}$ .

With  $I_p \simeq 10 \text{ A}$ ,  $\tau_p \simeq 1 \text{ ps}$ ,  $\varepsilon_n \simeq 10^{-7} \text{ m rad}$ :

Gain  $G > 15 \%$  is feasible

# X-FEL Oscillator Principles



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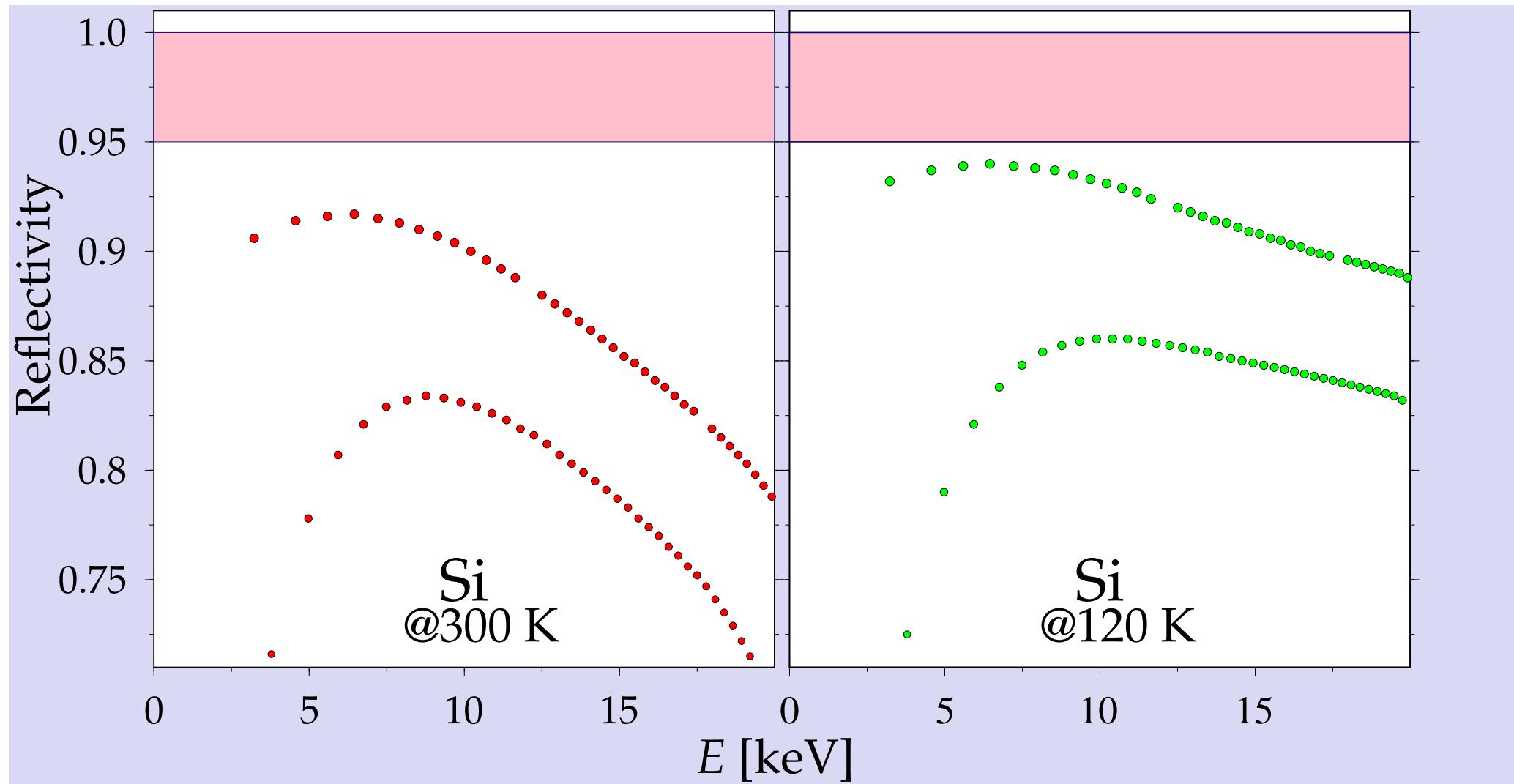
Small gain requires

low-loss optical cavity:

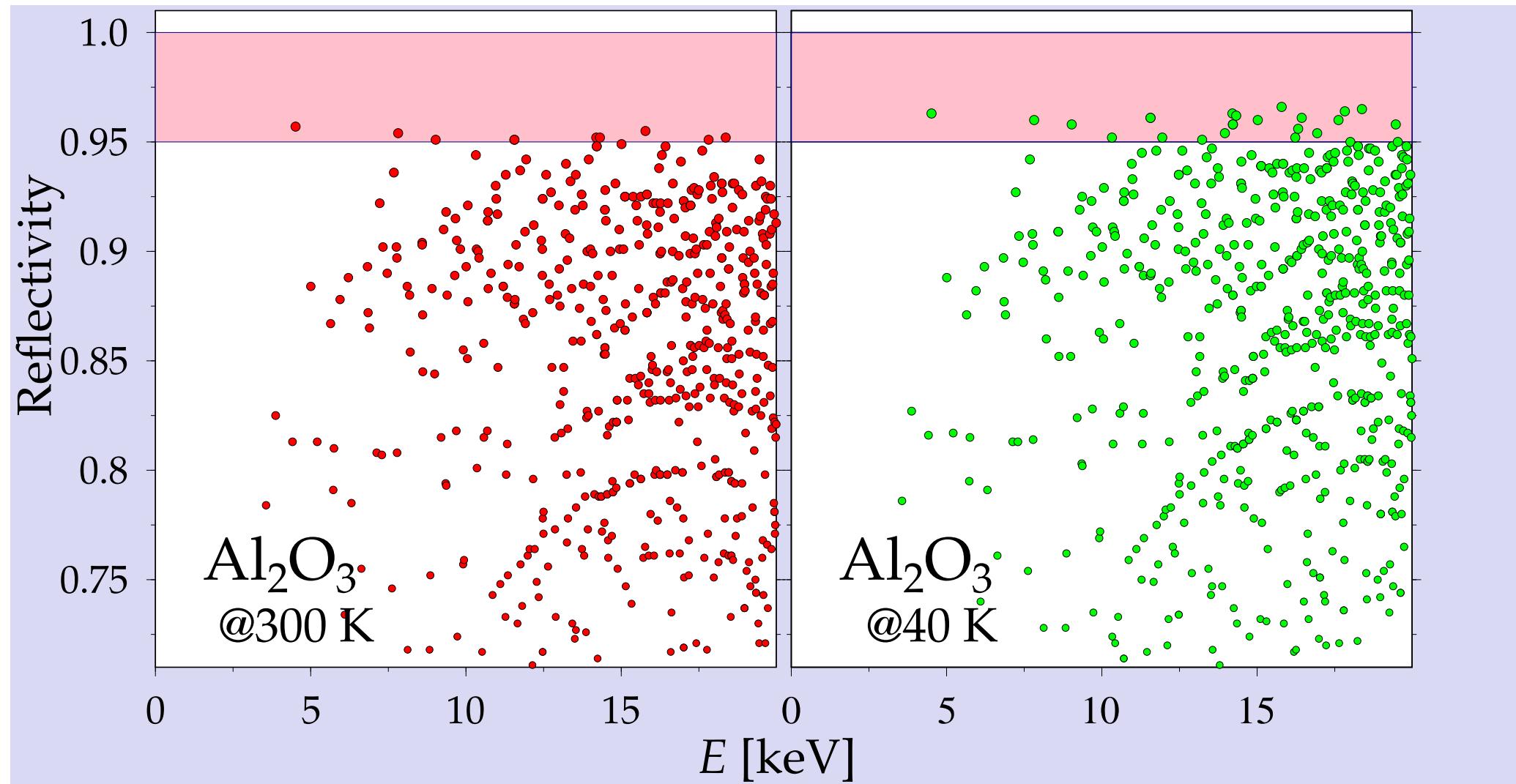
$$R_1 \times R_2 > 90\%$$

$$R_1, R_2 > 95\%$$

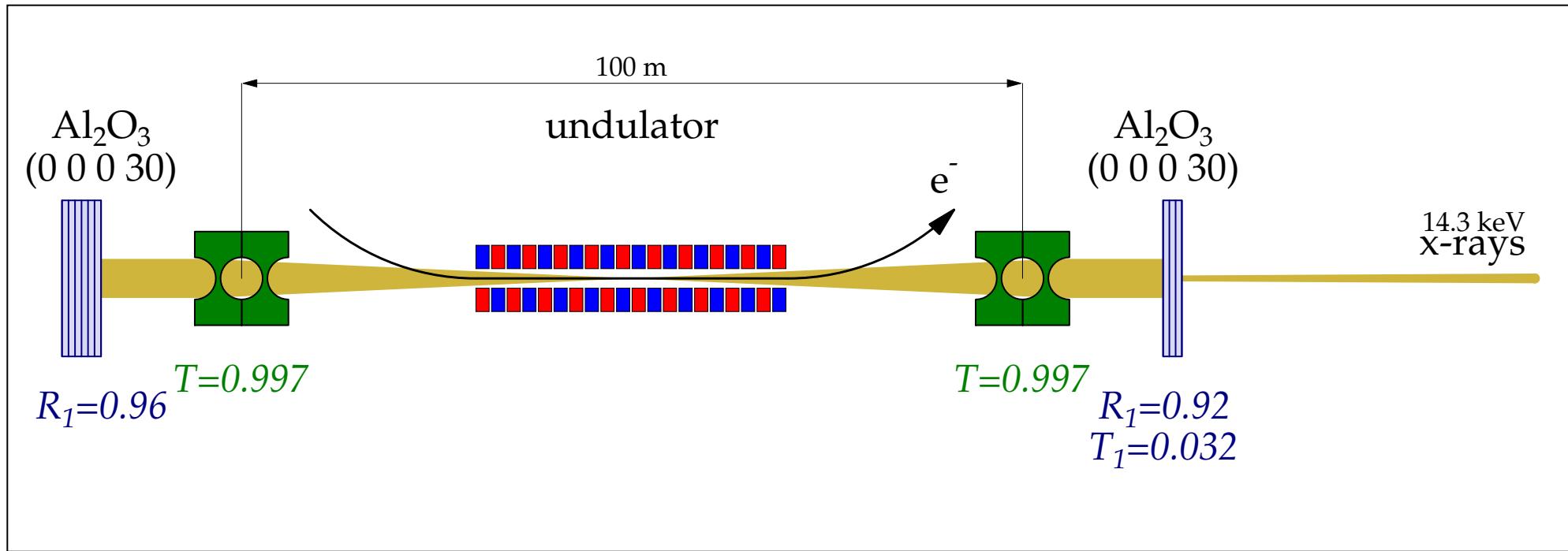
# Reflectivity of Si in backscattering



# Reflectivity of sapphire in backscattering



# Sapphire cavity with CRL



$$R_1 \times R_2 \times T^4 = 0.87$$

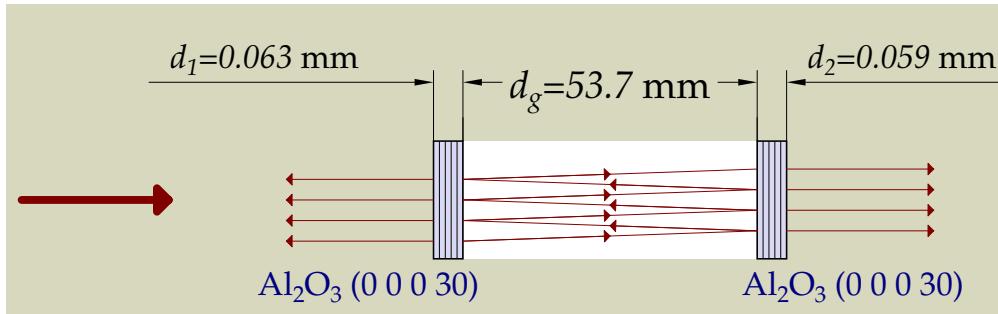
$$T_1 \simeq 0.032$$

CRL:  $F = R/2N\delta = 50$  m

[ $R = 0.333$  mm;  $N = 2$ ;  $\delta = 1.6 \times 10^{-6}$ ]

B. Lengeler, C. Schroer, et al, JSR 6 (1999) 1153

# Sapphire X-ray resonator demonstrated

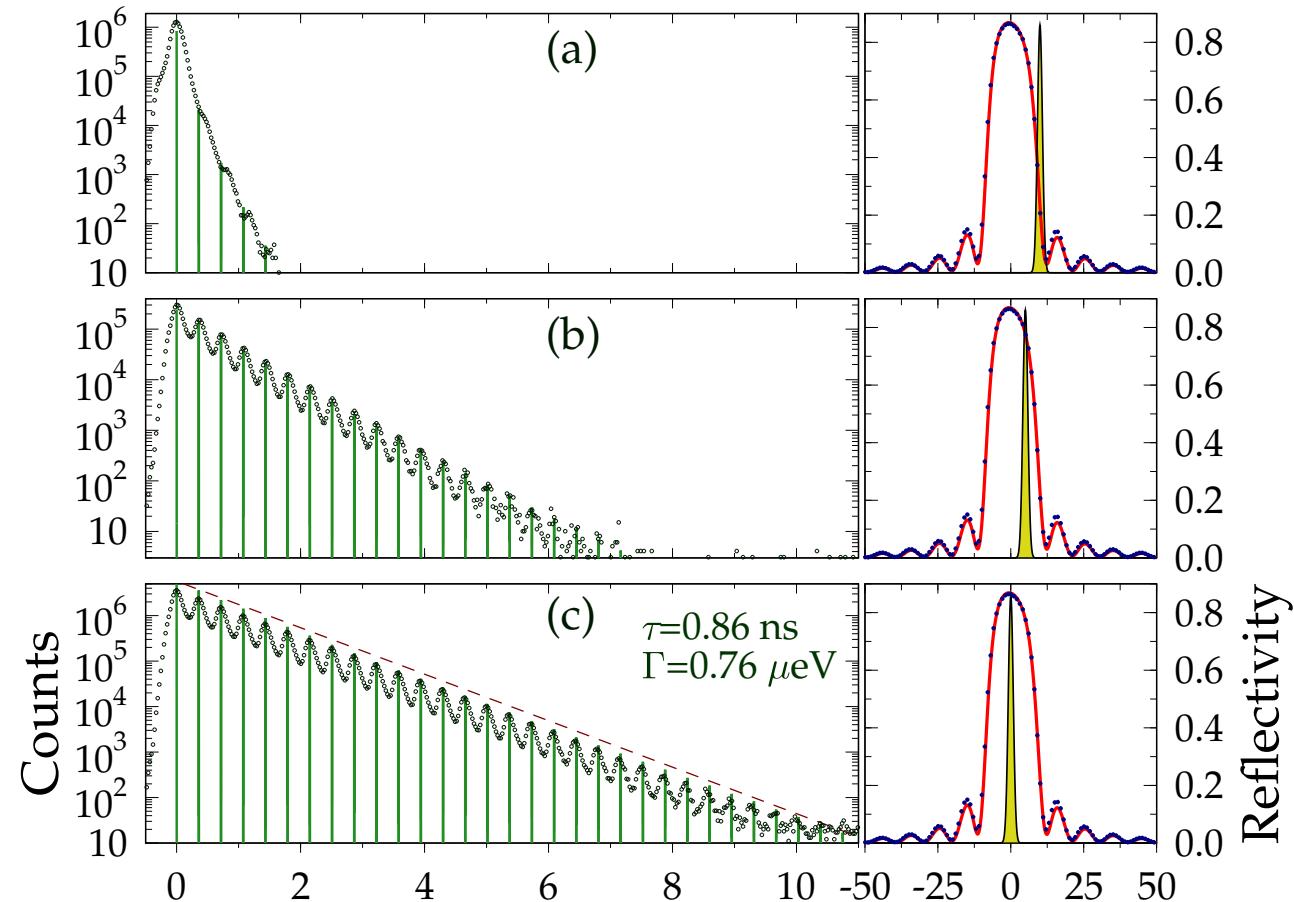


Shvyd'ko, Lerche, Wille et al, *PRL* **90** (2003) 013904

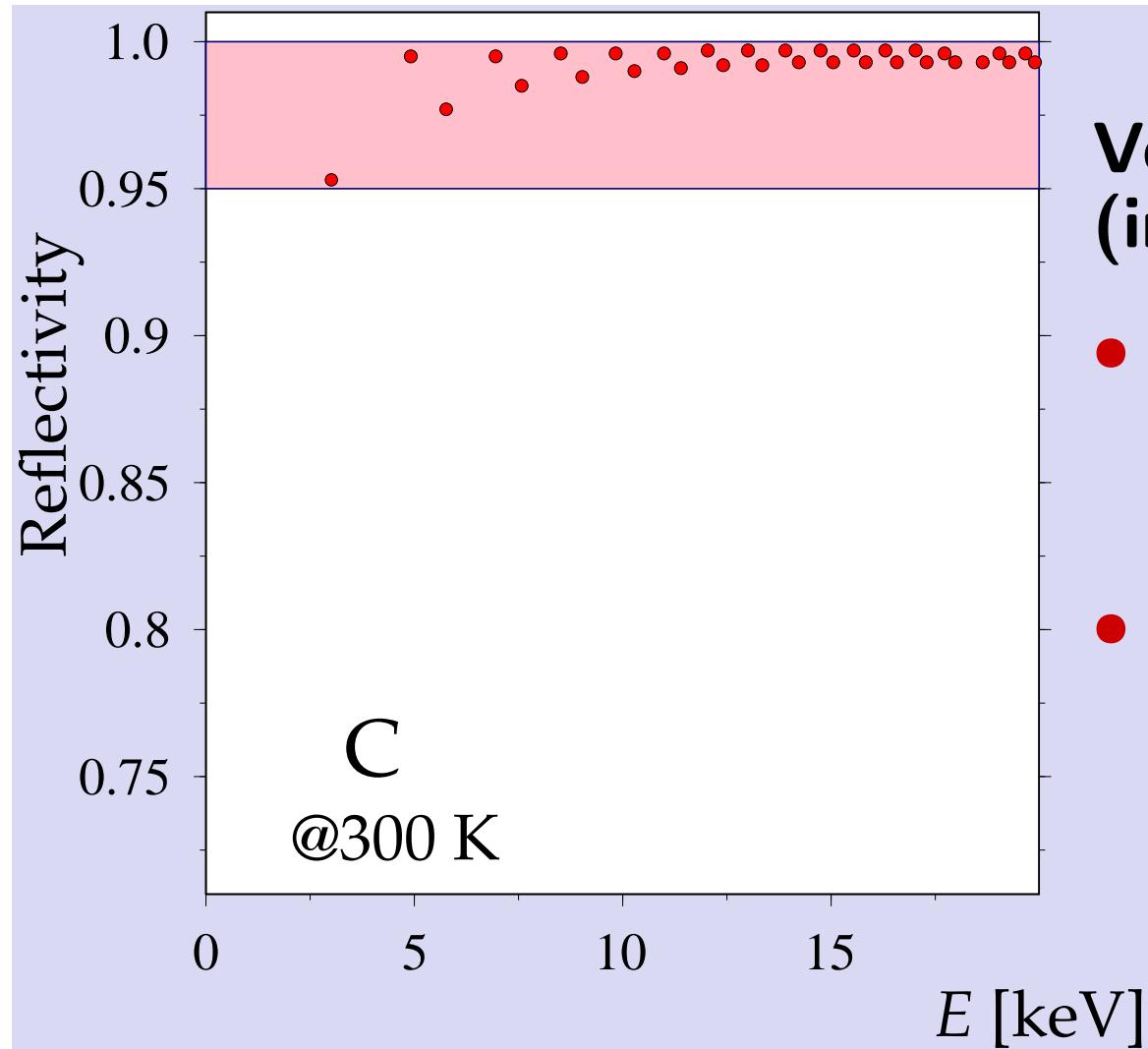
Measured finesse = 15

Measured reflectivity = 0.82

Expected reflectivity = 0.86



# Reflectivity of diamond in backscattering

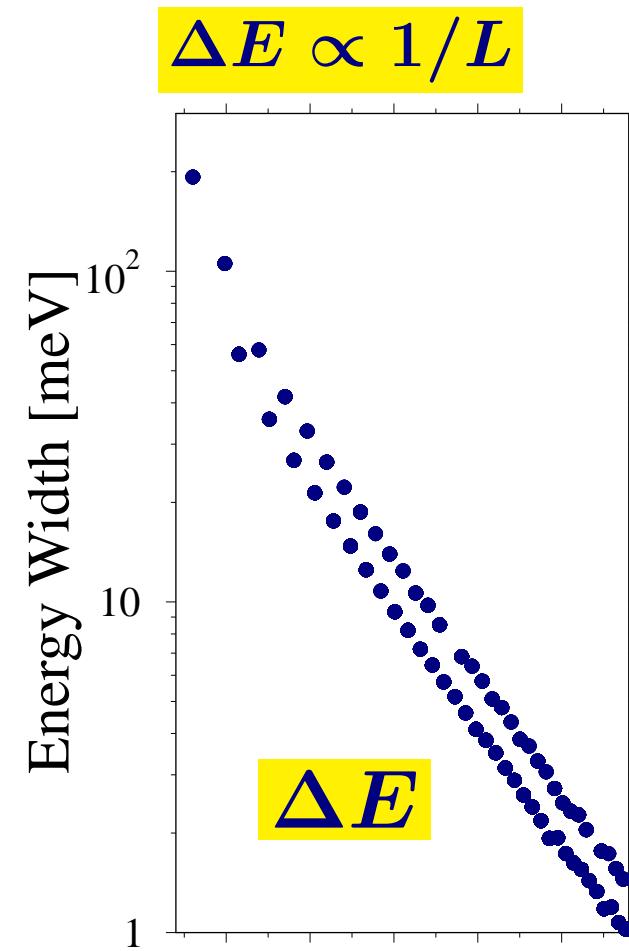
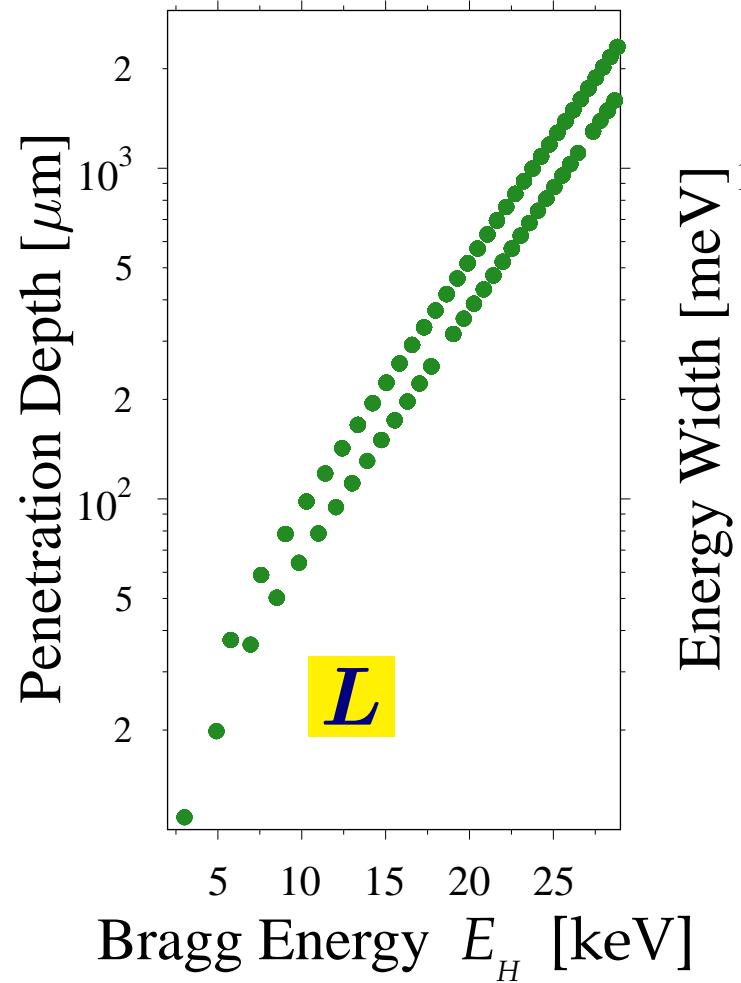
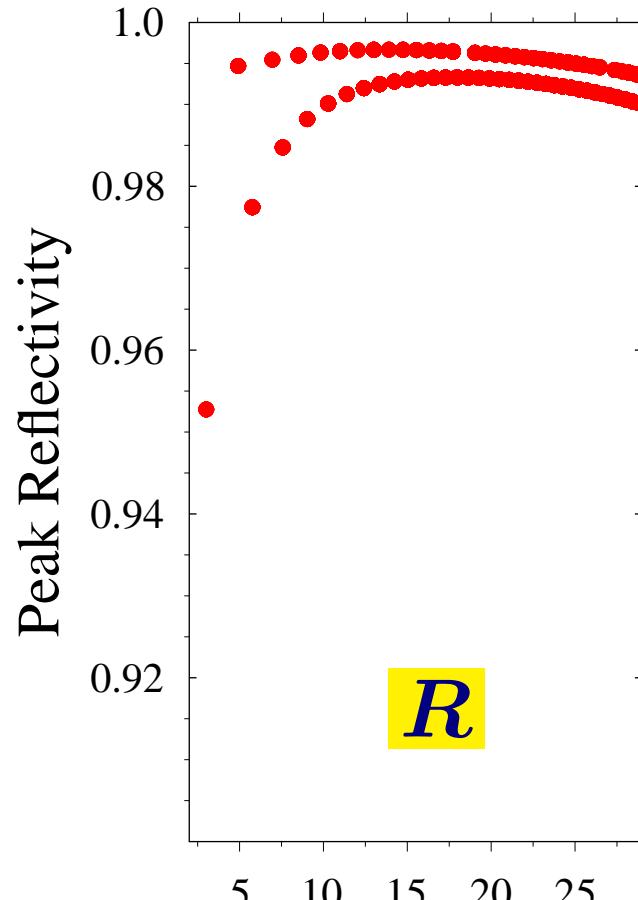


Very high reflectivity  
(in theory) due to:

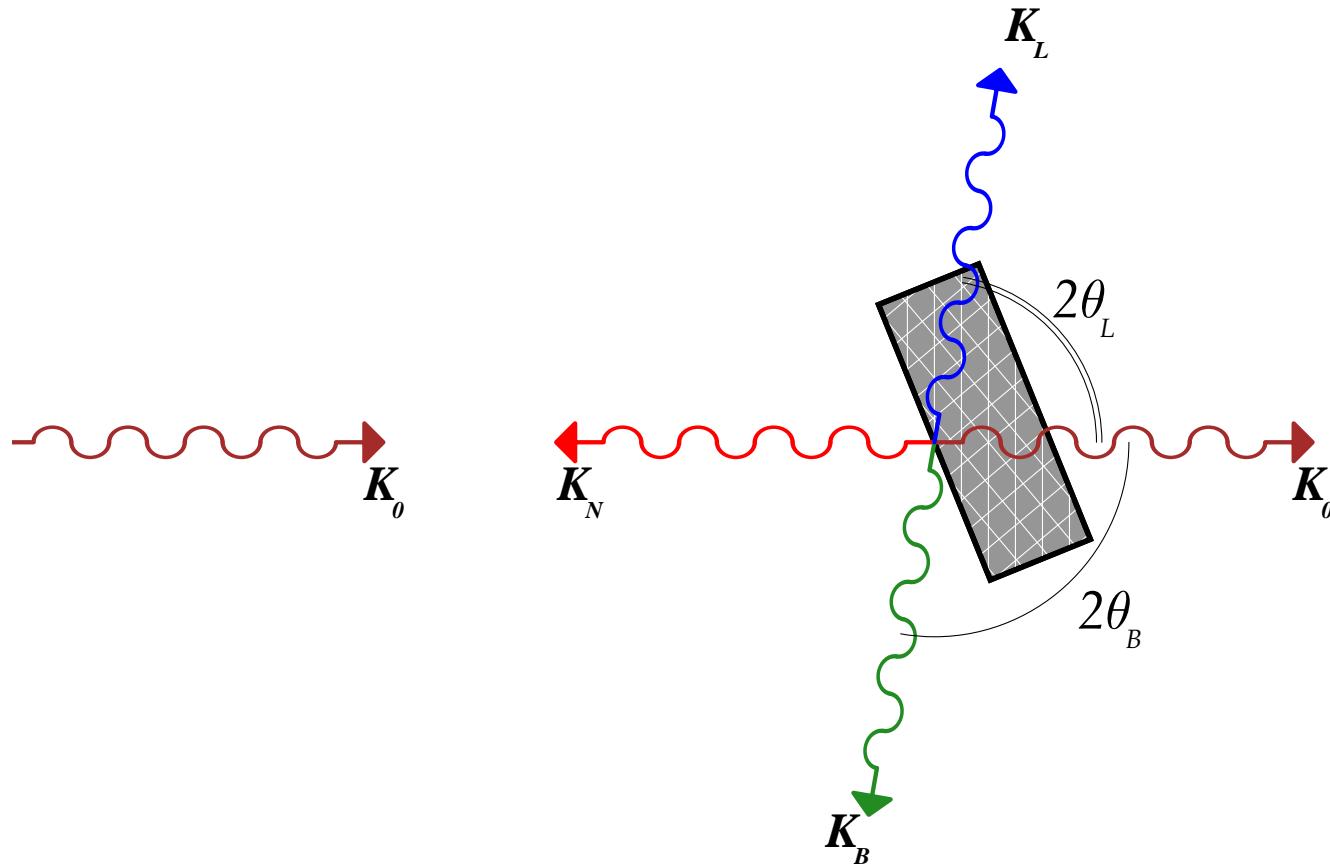
- High Debye Temperature, and thus high Debye-Waller factor
- Low  $Z$ , low photo absorption

# Reflectivity vs. Penetration & Energy Width

$R$ ,  $L$ , and  $\Delta E$  are interconnected.



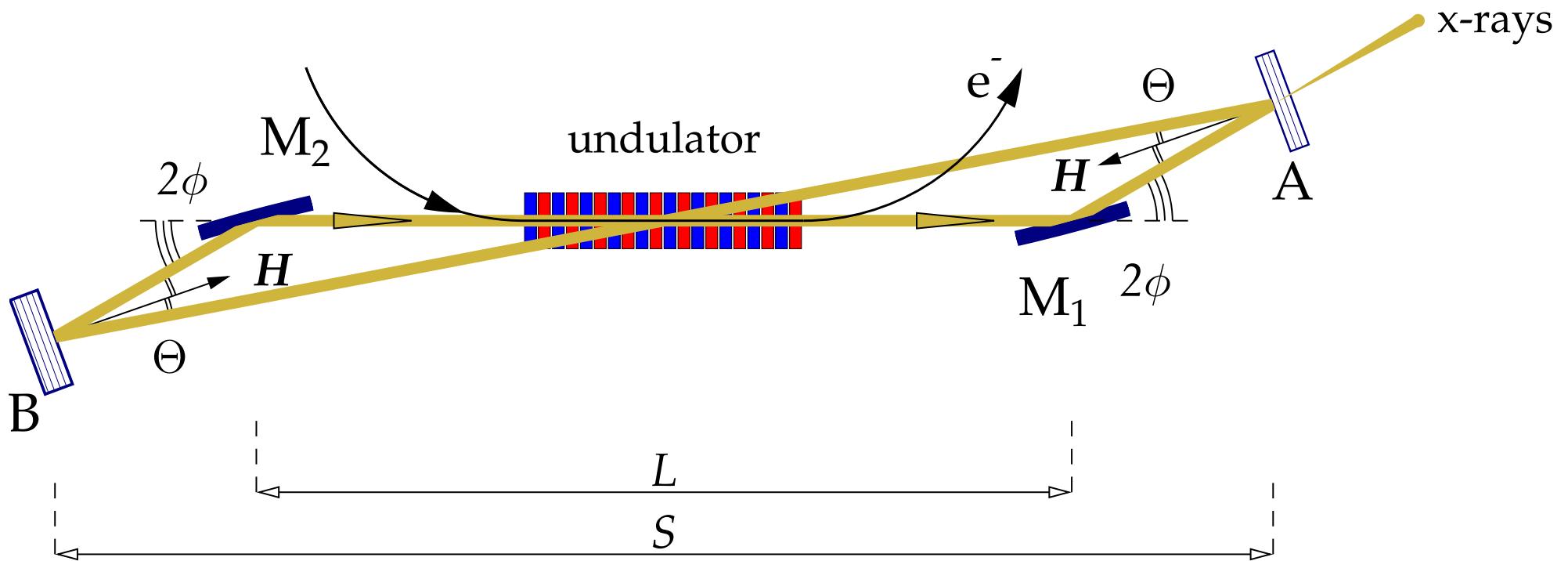
# Multiple-beam Bragg Diffraction in Backscattering



Bragg-reflection condition can be fulfilled simultaneously for more than one reflecting atomic plane. In backscattering from Si, C, crystal this happens for all Bragg reflections except (111) and (220).

**Si and C are not favorable as X-ray exact-backscattering mirrors**

# Diamond cavity for the X-FEL Oscillator

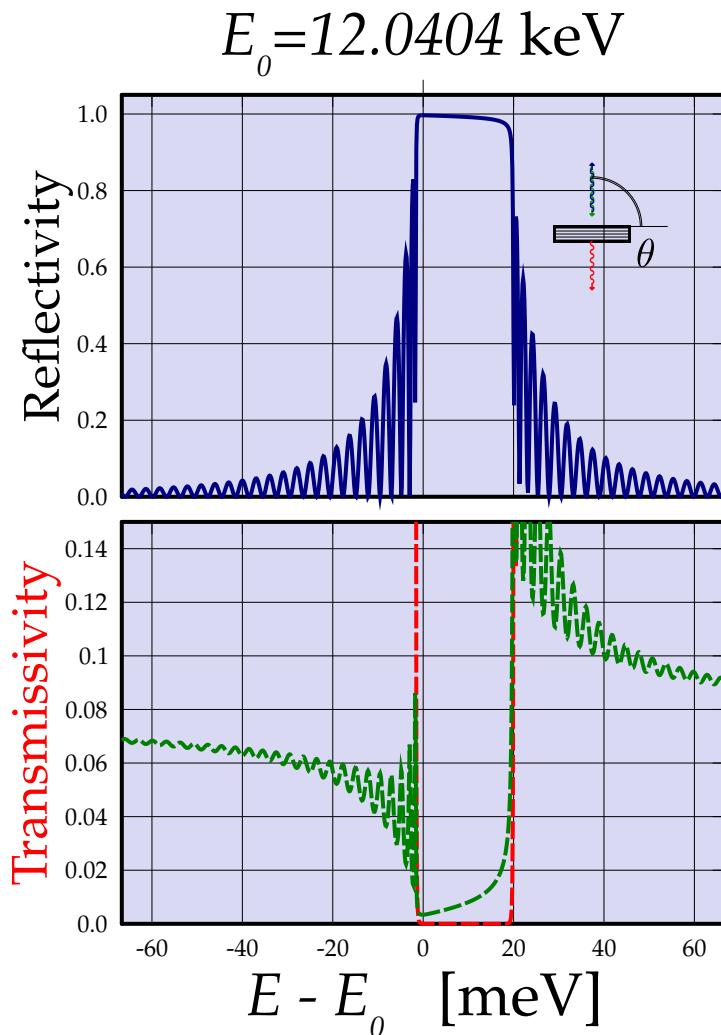


$$R_A \times R_B \times R_{M_1} \times R_{M_2} \simeq 0.9$$

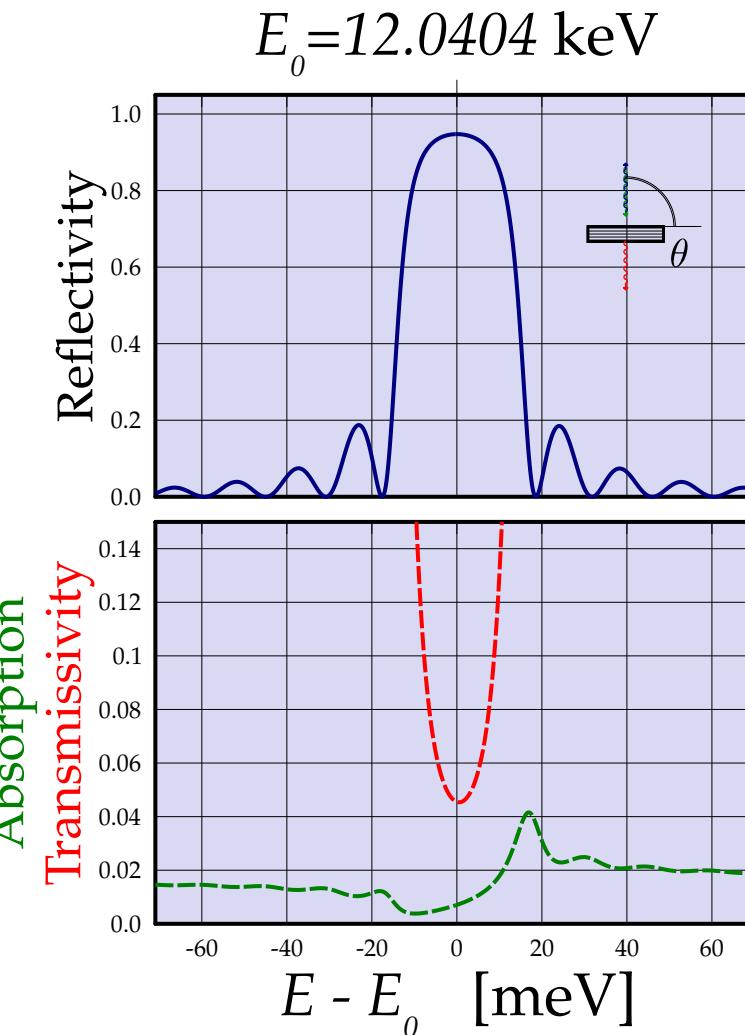
$$T_A \simeq 0.04$$

# Diamond crystal and mirror reflectivity @ 12 keV

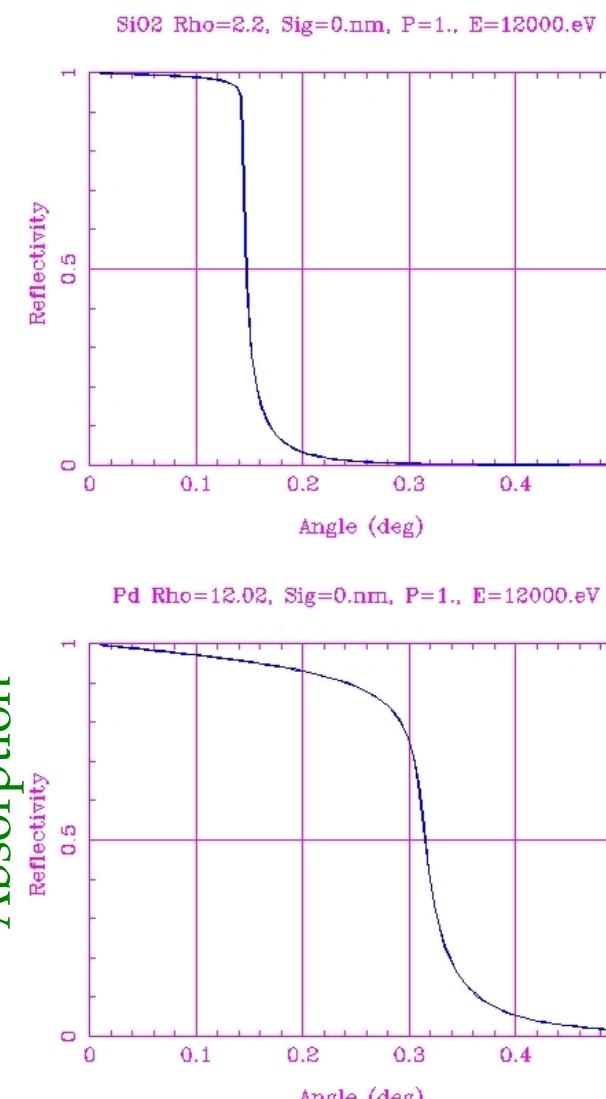
Narrow band mirrors:  $\Delta E \approx 10 \text{ meV}$ ;  $\Delta E \approx \hbar/\tau_p$



$C(4\ 4\ 4)$ ;  $L = 0.2 \text{ mm}$ ;  $T = 300 \text{ K}$   
bradix version: January, 2007

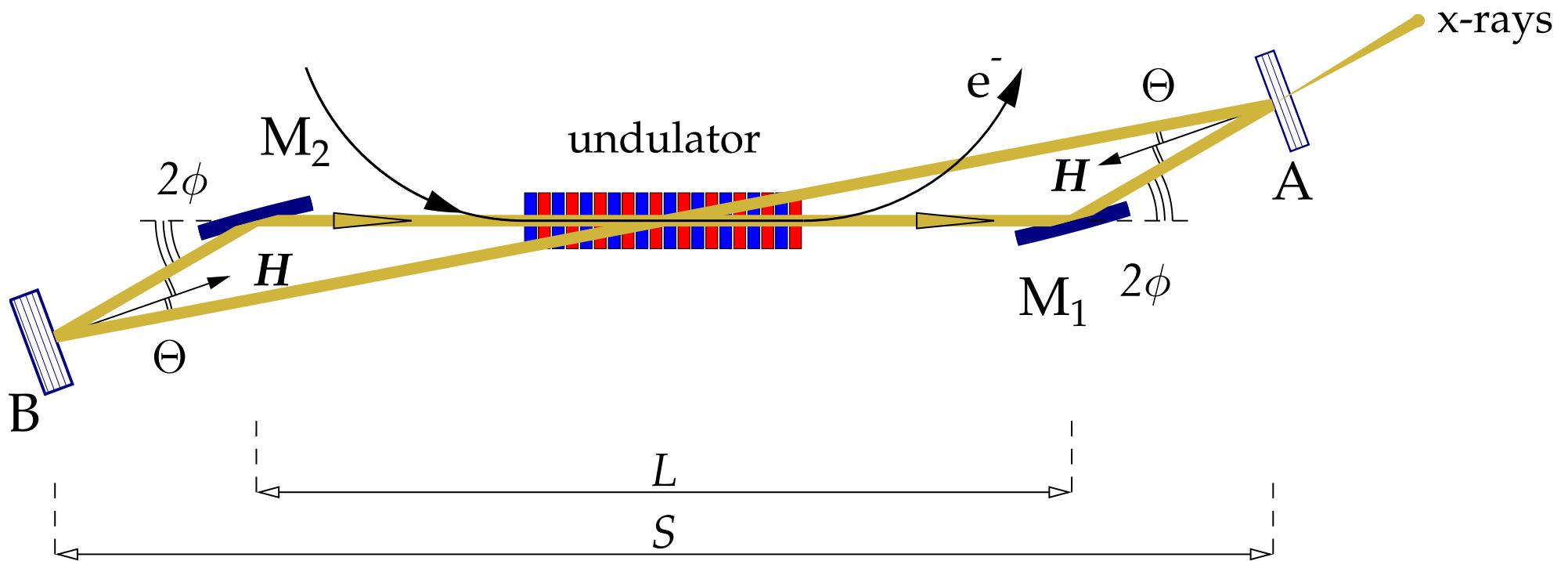


$C(4\ 4\ 4)$ ;  $L = 0.042 \text{ mm}$ ;  $T = 300 \text{ K}$   
bradix version: January, 2007



Mirror calculations:  
[www-cxro.lbl.gov](http://www-cxro.lbl.gov)

# Two-Crystal Cavity is not Tunable

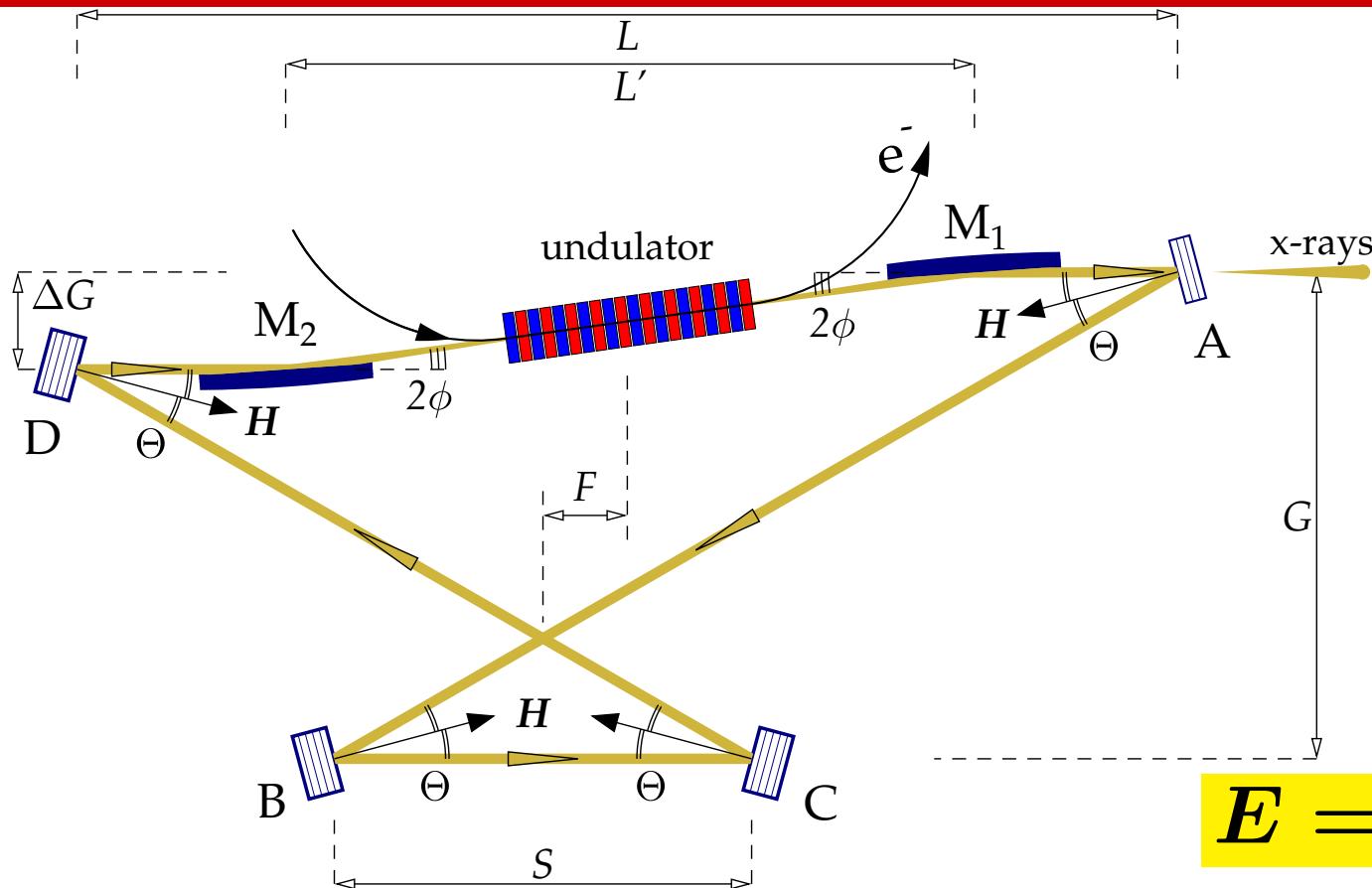


$E = E_H \cos \Theta \Rightarrow$  Two-crystal scheme is not tunable.

Because, it is necessary to keep small  $\phi \lesssim 2$  mrad

and therefore small  $\Theta \lesssim 2$  mrad, for high reflectivity of the mirrors.

# Tunable Cavity



A four-crystal (**A,B,C, and D**) x-ray optical cavity allows photon energy  **$E$**  tuning in a broad range by changing the incidence angle  **$\Theta$** .

R.M.J. Cotterill, Appl. Phys. Lett., 12 (1968) 403

K.-J. Kim, and Yu. Shvyd'ko, Phys. Rev. STAB (2009)

# XFELO Simulations

R. Linberg, K.-J. Kim, W. Falley, Yu. Shvyd'ko

■ Undulator:

$$\lambda_u = 1.76 \text{ cm} \quad K = 1.5$$

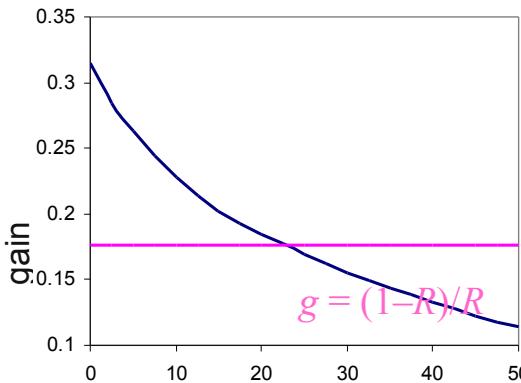
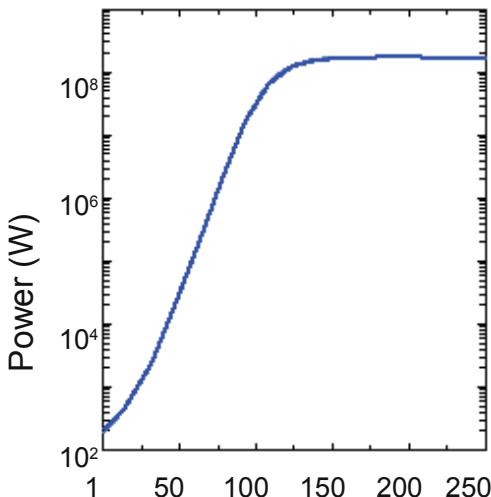
■ Electron beam:

$$I = 10\text{A} \quad \epsilon_x = 2 \times 10^{-7} \quad \beta_x = 10 \text{ m}$$

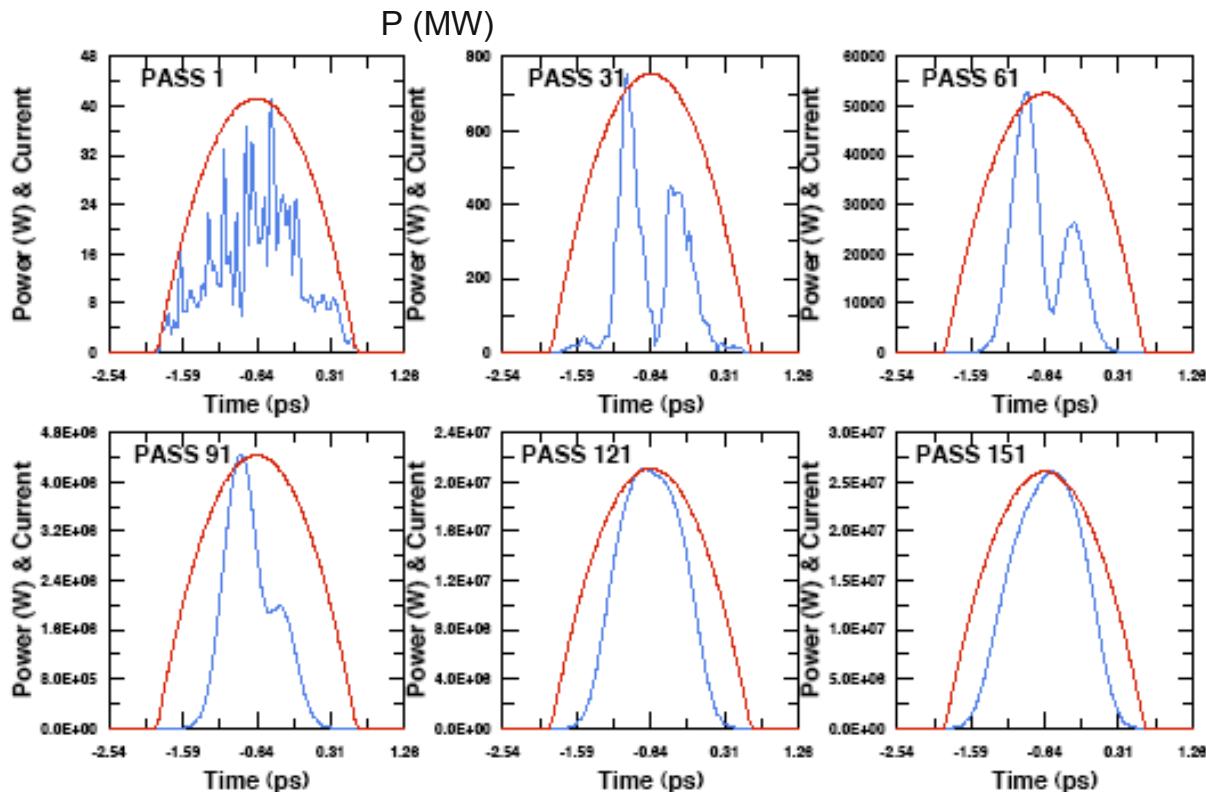
■ Bragg crystal:

Diamond,  $\tau_M \approx 100 \text{ fs}$

GINGER simulation shows evolution from noise to power levels near those expected

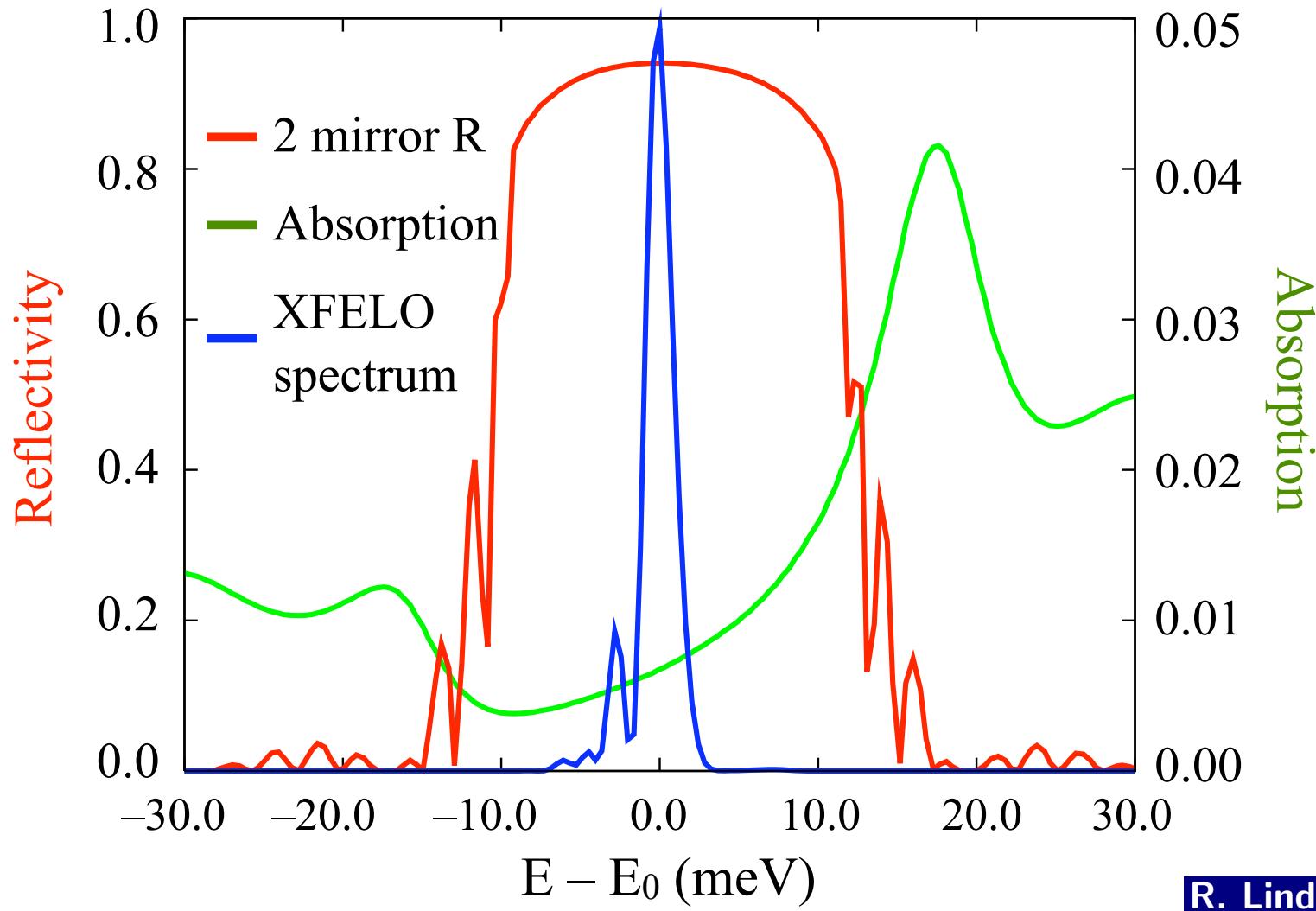


Single slice gain calculations indicate saturation power ~23 MW for mirror losses = 85%



# XFELO Spectrum

After 500 passes in 2-crystal diamond cavity:



# XFEL-O Performance

---

- Photon spectral range:  $2 \lesssim E \lesssim 25$  keV.
- Full transverse and temporal coherence of  $\approx 1$  ps (rms)  $\Rightarrow \Delta E \simeq 2$  meV.
- $5 \times 10^8$  photons/pulse (1  $\mu$ J/pulse)
- Peak spectral brightness comparable to SASE XFEL.
- Repetition rate  $\gtrsim 1.5$  MHz  $\Rightarrow (7.5 \times 10^{14} \text{ ph/s} = 1.7 \text{ W})$  average spectral brightness factor  $\simeq 10^5$  larger than SASE XFEL, and comparable to the seeded SASE XFEL.
- Being operated at 14.4 keV, XFEL-O would generate  $\approx 10^3$  Mössbauer photons per pulse with a 5 neV spectral width, the natural width of the 14.4 keV nuclear resonance in  $^{57}\text{Fe}$ . With a repetition rate of  $\gtrsim 10^6$  Hz, the XFEL-O would produce about  $10^9$  fully coherent 14.4 keV Mossbauer photons per second.
- Tunable.

# Science drivers for XFEL-O

---

Many x-ray spectroscopies and techniques require hard x-rays ( $E \gtrsim 2$  keV) with very narrow energy bandwidth  $\Delta E \lesssim 1$  meV i.e. temporal coherence  $\gtrsim 1$  ps:

- Inelastic x-ray scattering (IXS).
- Nuclear resonant scattering (NRS).
- HAXPES (hard-xrays photoemission spectroscopy).
- Imaging with hard x-rays at near-atomic resolution ( $\simeq 1$  nm).
- Time-resolved (ps) measurements (structure, dynamics).
- Metrology: Mössbauer wavelength standard for atomic scales.
- etc, etc.

# Technical Challenges

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## Ultra-low emittance injector.

### X-ray Optics:

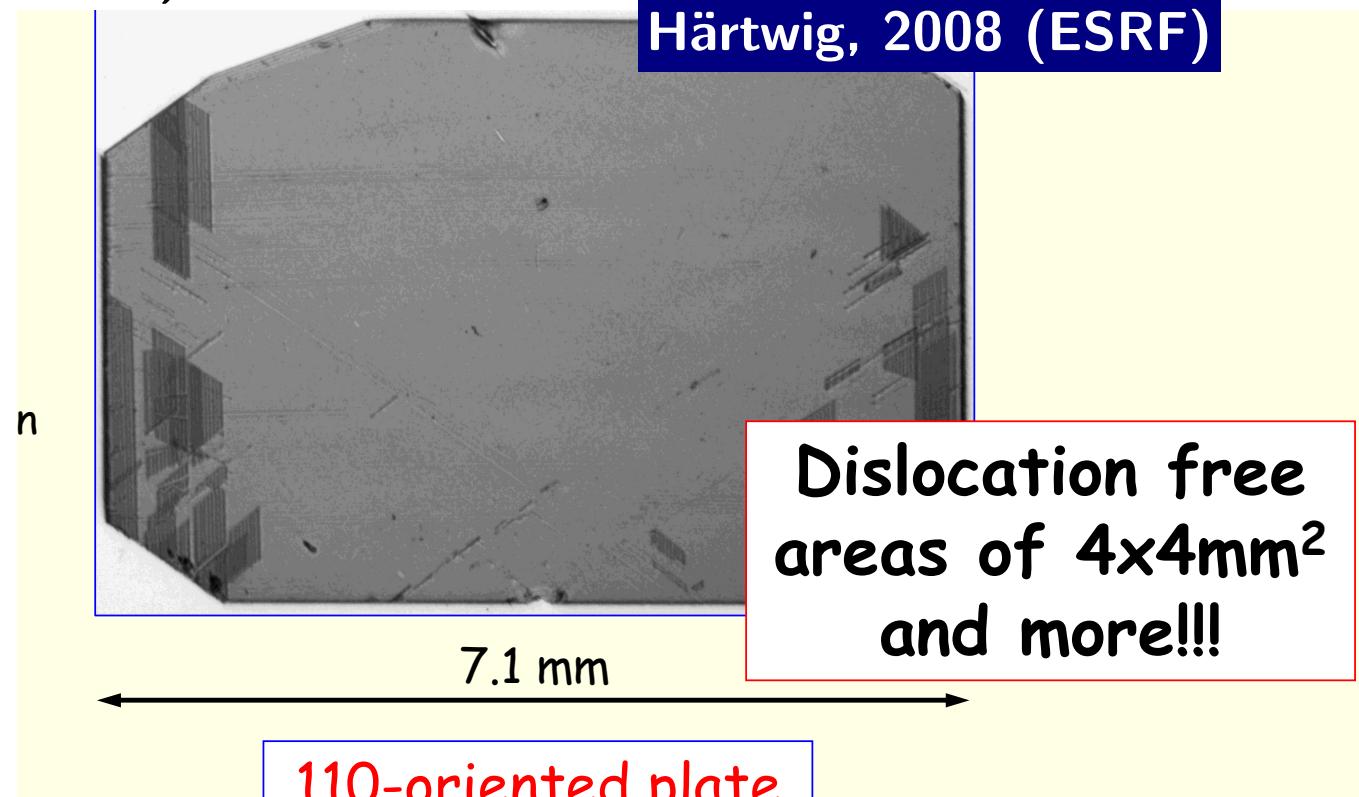
- **Quality of diamond crystals:**  
is the theoretical reflectivity achievable?
- **Heat load problem (reflection region variations  $\lesssim 1 \text{ meV}$ ).**
- **Angular stability:**  $\delta\theta \lesssim 10 \text{ nrad}$

Spatial stability:  $\delta L \lesssim 3 \text{ } \mu\text{m} \text{ (rms)} \rightarrow \delta L/L \lesssim 3 \times 10^{-8}$

# Quality of Diamond crystals

## Required diamond crystals:

- high quality (dislocation free, etc.)
- thin:  $\lesssim 200 \mu\text{m}$
- small suffice:  $\simeq 1 \text{ mm}^2$



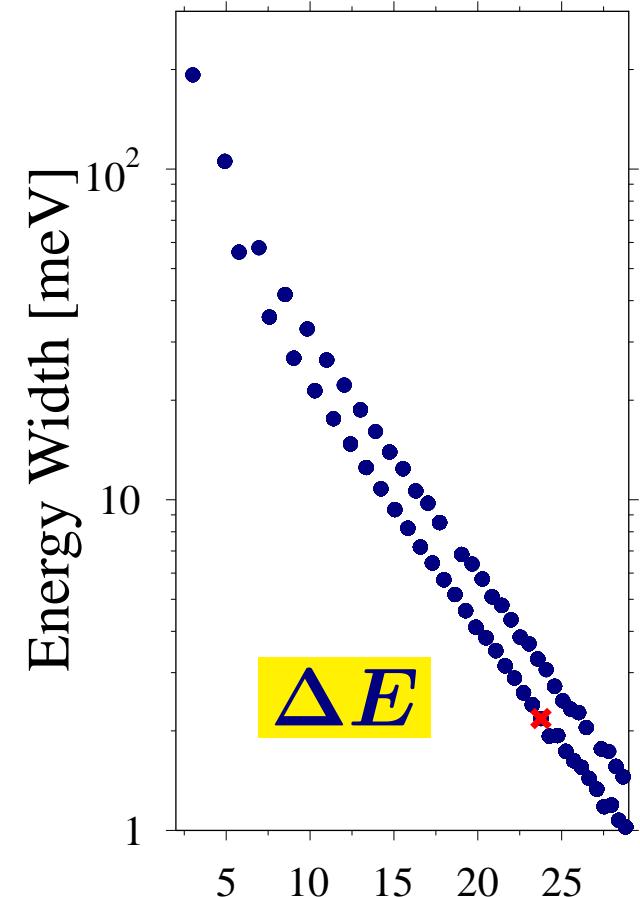
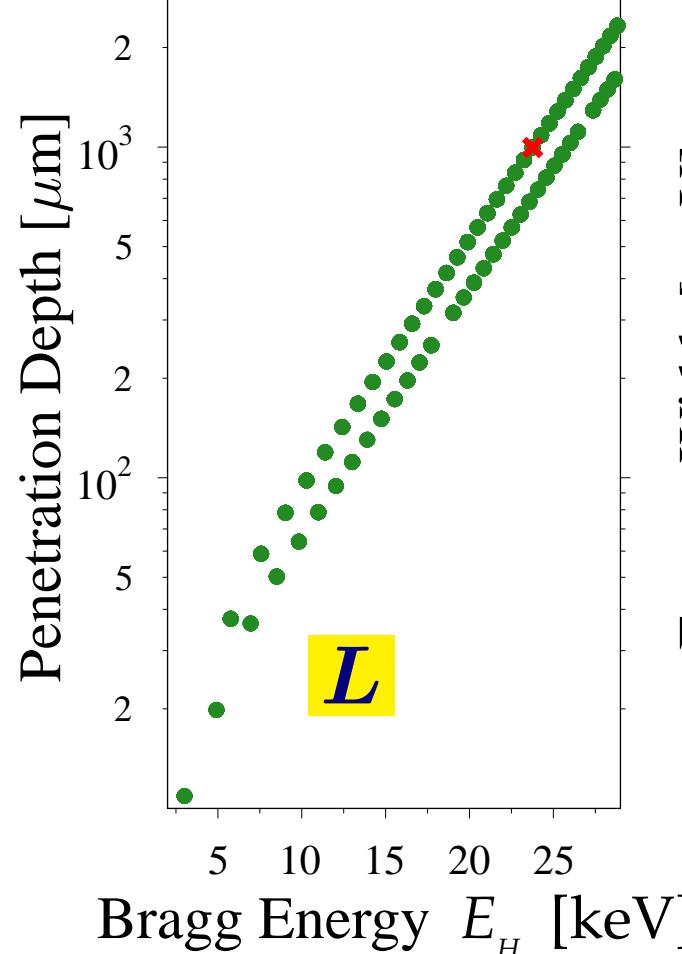
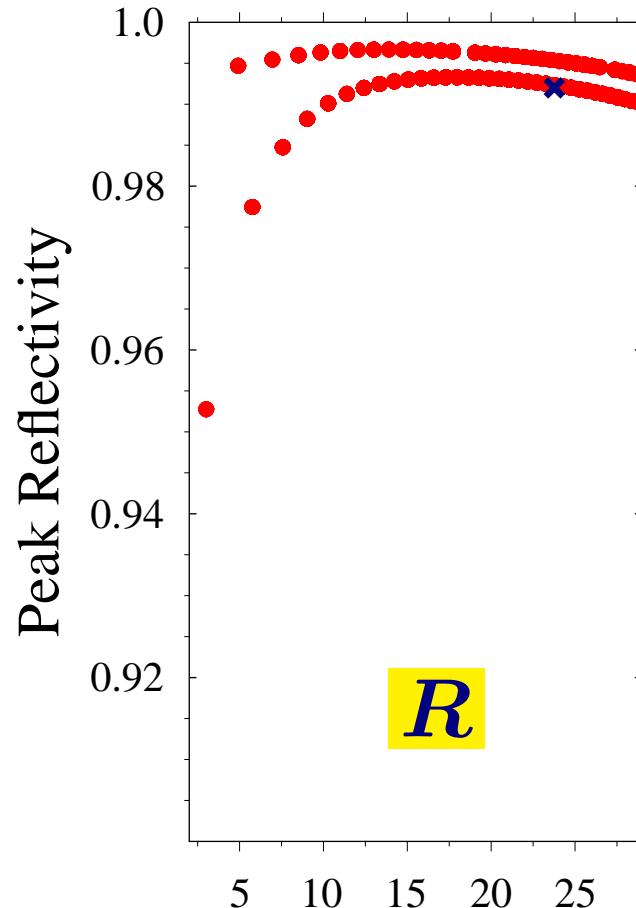
Still open question:  
is the theoretical reflectivity achievable?

White beam topograph in transmission

# Reflectivity vs. Penetration & Energy Width

$R$ ,  $L$ , and  $\Delta E$  are interconnected.

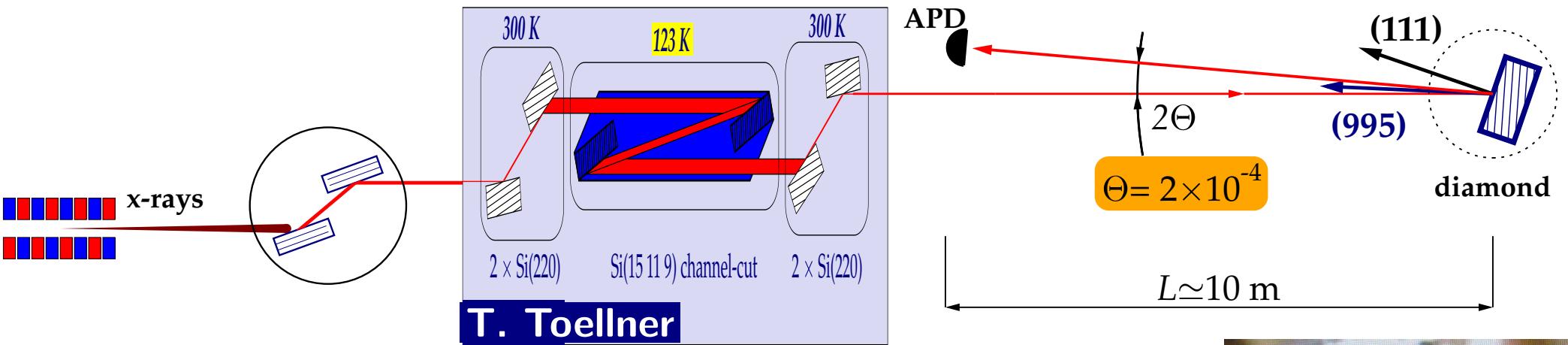
$\Delta E \propto 1/L$



Smallness of  $\Delta E$  is a hallmark of high quality crystal

# Experiment, Sector 30 @ APS, March 2009

S. Stoupin, Yu. Shvyd'ko, A. Cunsolo



T. Toellner

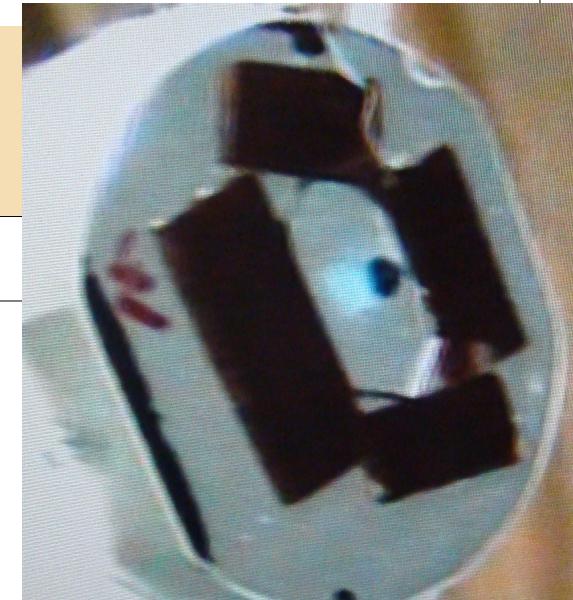
undulator

C(111) cooled  
monochromator

bandwidth  
 $\approx 100 \text{ eV}$

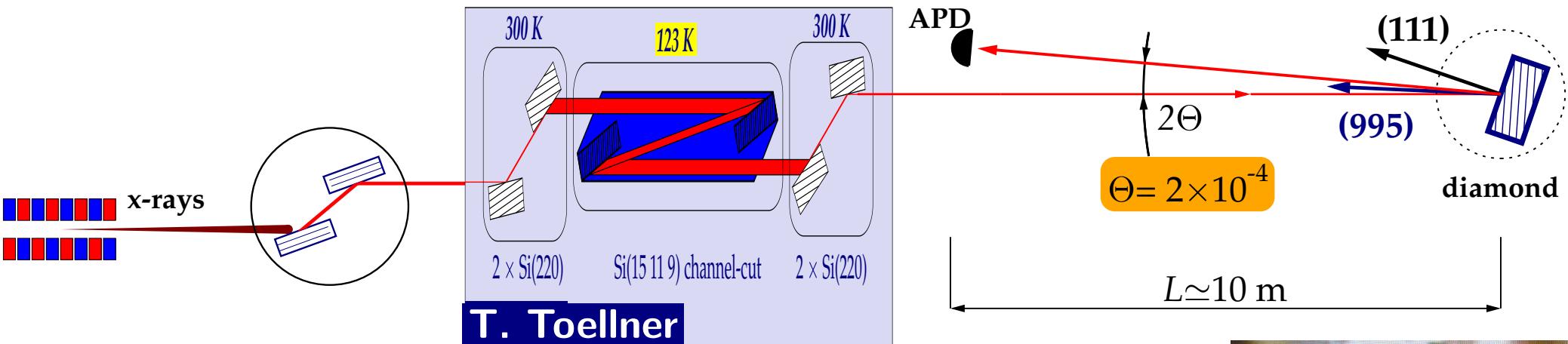
high-resolution  
monochromator  
 $E=23.7 \text{ keV}$

**bandwidth**  
 $\Delta E \approx 1 \text{ meV}$



# Experiment, Sector 30 @ APS, March 2009

S. Stoupin, Yu. Shvyd'ko, A. Cunsolo



T. Toellner

undulator

C(111) cooled  
monochromator

high-resolution  
monochromator  
 $E=23.7$  keV

bandwidth  
 $\approx 100$  eV

bandwidth  
 $\approx 1.7$  eV

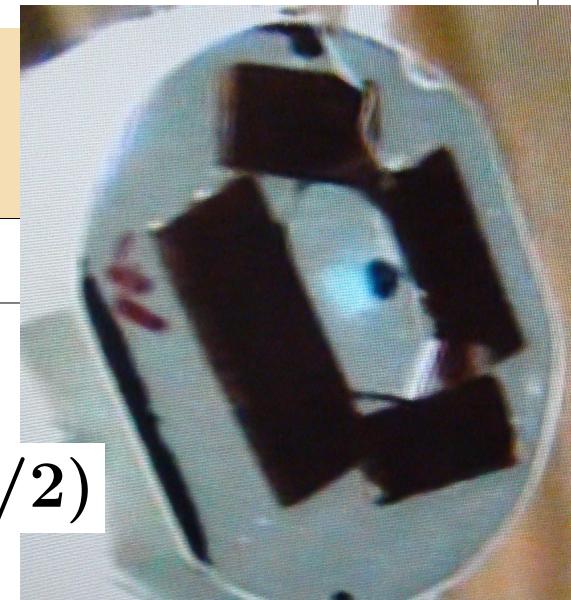
bandwidth  
 $\Delta E \approx 1$  meV

**Bragg's law:**  $\lambda = 2d \sin \theta$

$\theta = \pi/2 - \Theta$  ... in backscattering:  $\lambda = 2d(1 - \Theta^2/2)$

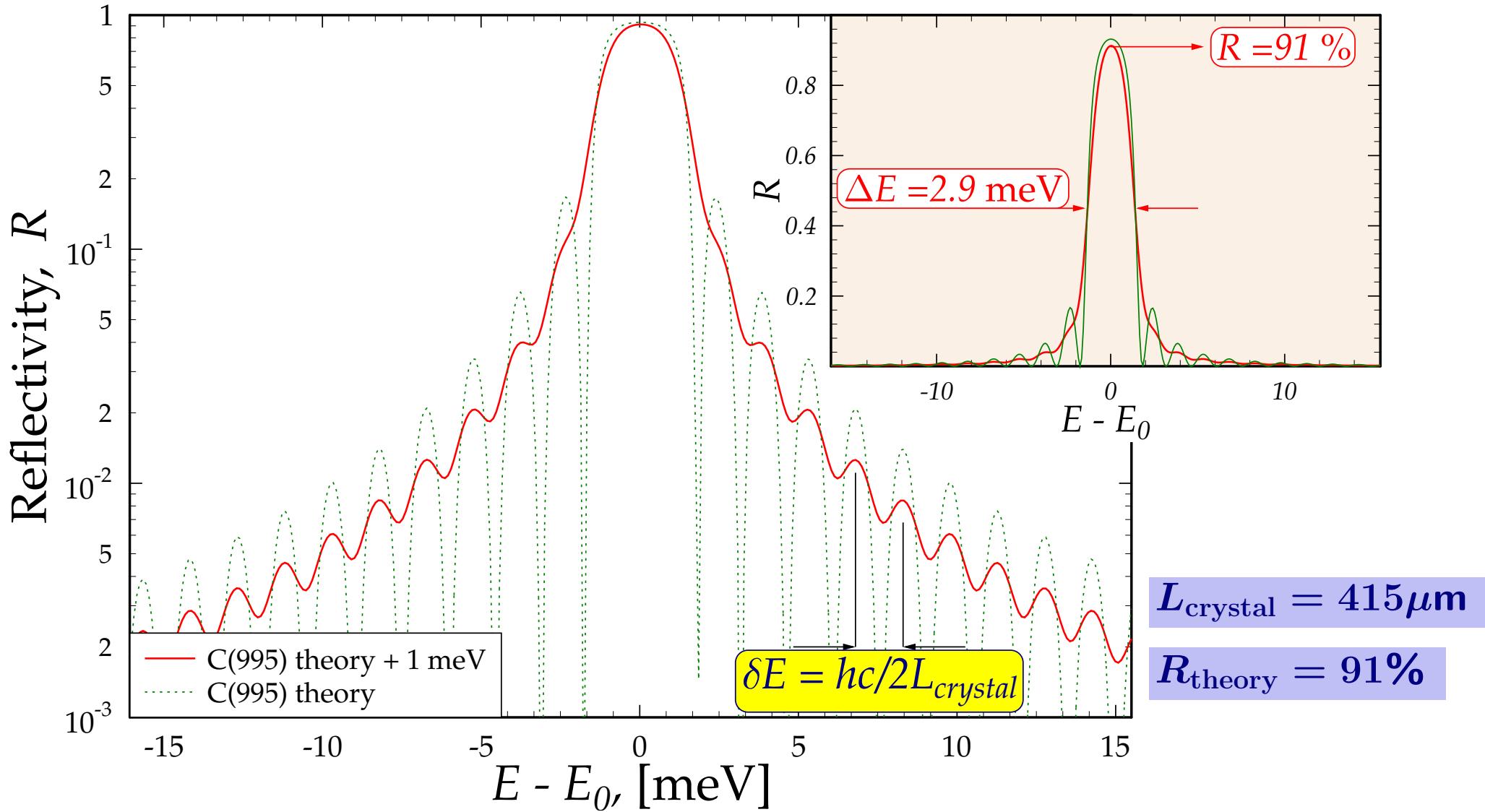
$E = E_H(1 + \Theta^2/2)$ ,  $E_H = hc/2d$

**Uncertainty:**  $\delta E/E_H = \Theta \delta \Theta \ll 10^{-8} \Rightarrow \delta E \ll 0.1$  meV



# Spectral Width and Reflectivity: Theory

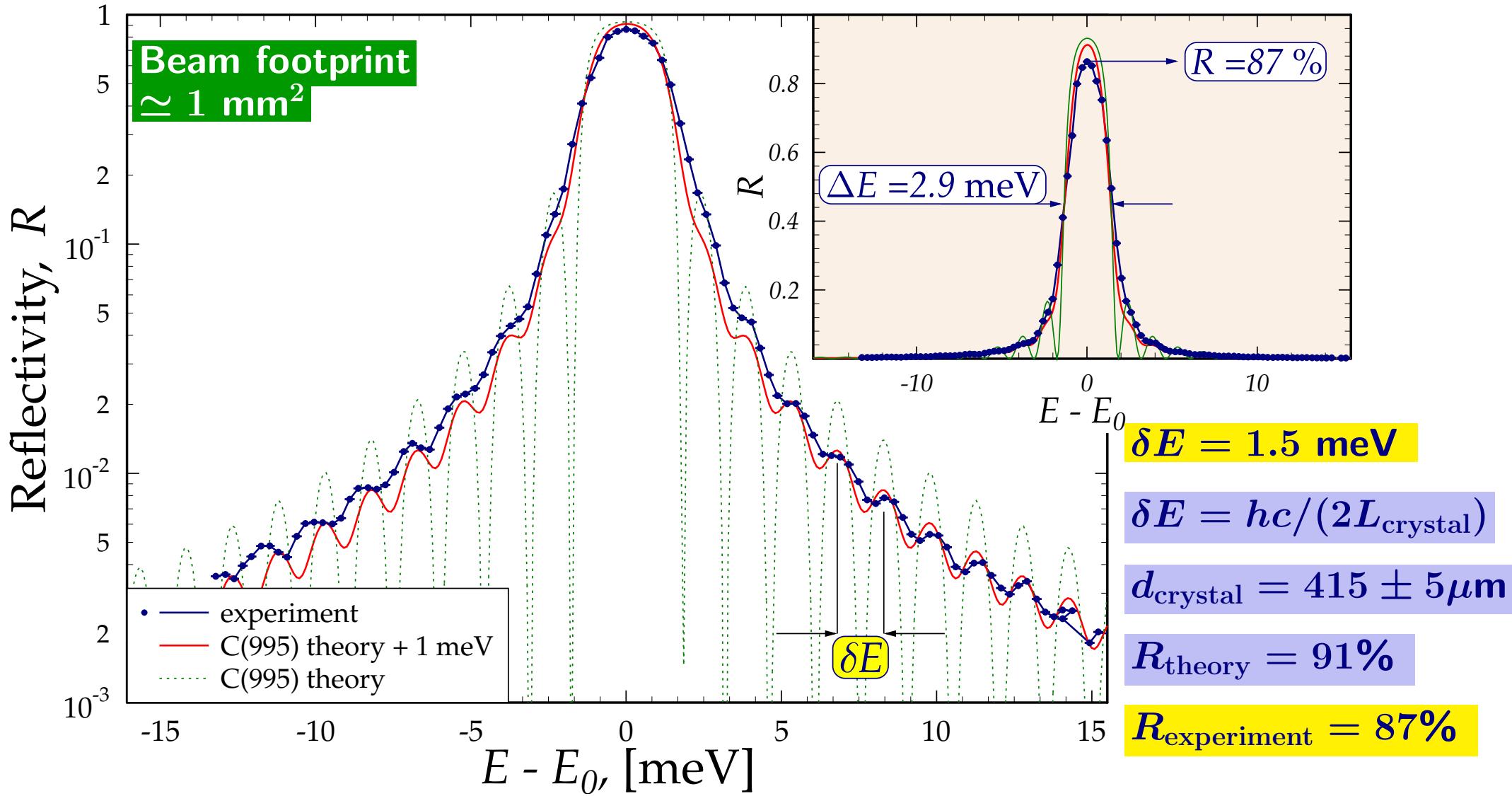
C(995),  $E_H = 23.765$  keV



# Spectral Width and Reflectivity: Experiment

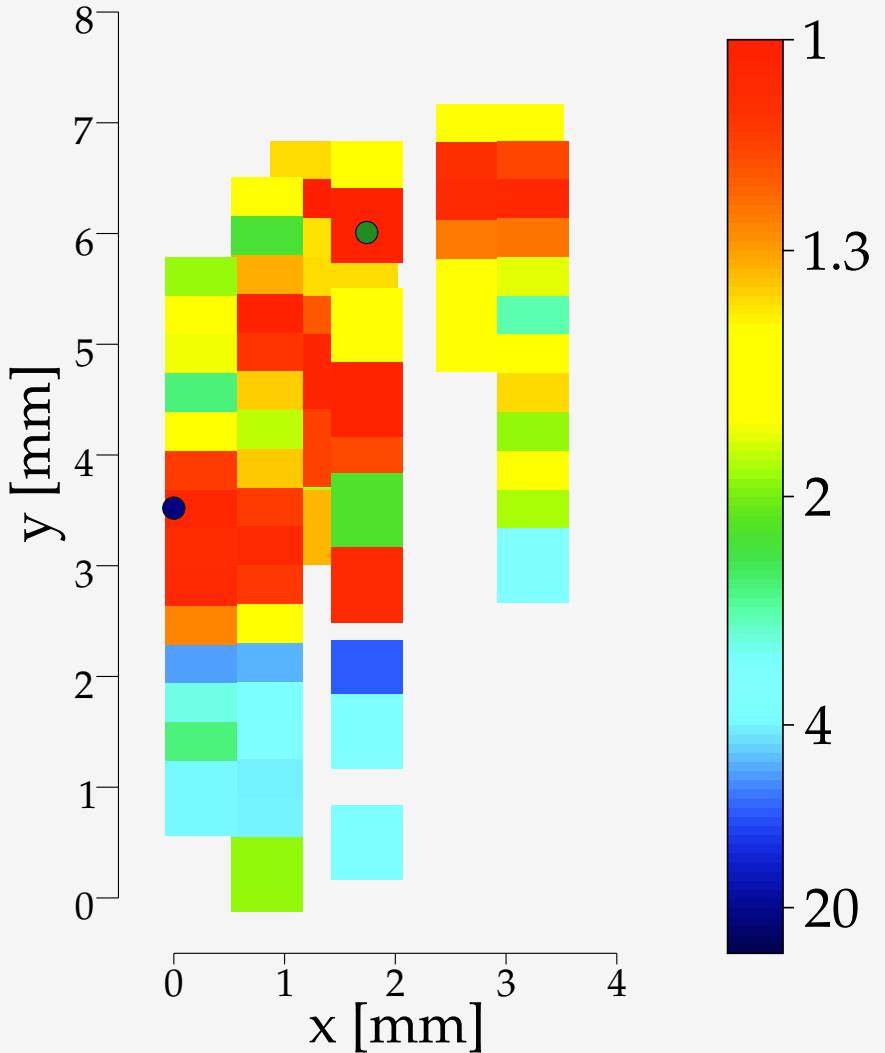
C(995),  $E_H = 23.765$  keV

Yu. Shvyd'ko, S. Stoupin, A. Cunsolo

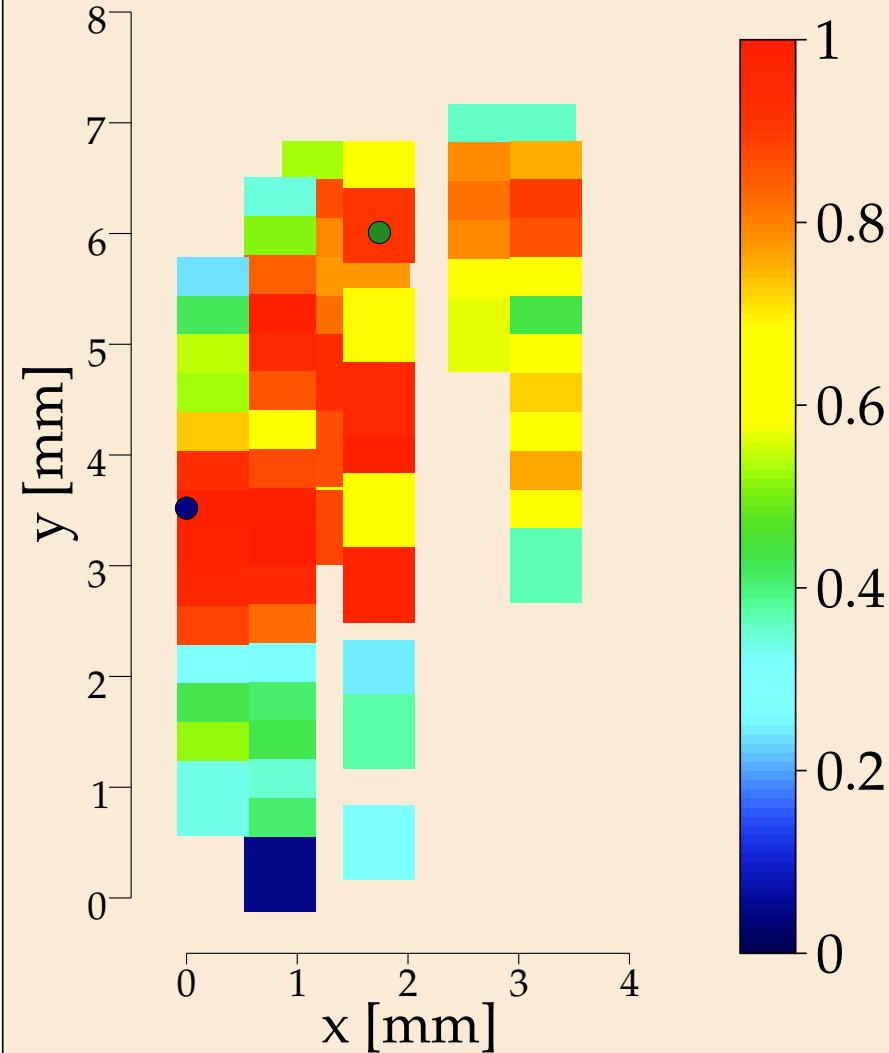


# Spectral Width and Reflectivity Measurements

Spectral width,  $\Delta E/\Delta E_{min}$



Reflectivity,  $R/R_{max}$



# Heat Load Problem

Temperature gradient  $\delta T \Rightarrow$  energy spread  $\delta E/E = \beta\delta T$ .

**Requirement:**  $\delta E \lesssim 1 \text{ meV}$ , when the next pulse arrives.

Incident power  $\simeq 50 \mu\text{J}/\text{pulse}$ .

Absorbed power:  $\simeq 1 \mu\text{J}/\text{pulse}$  (2%).

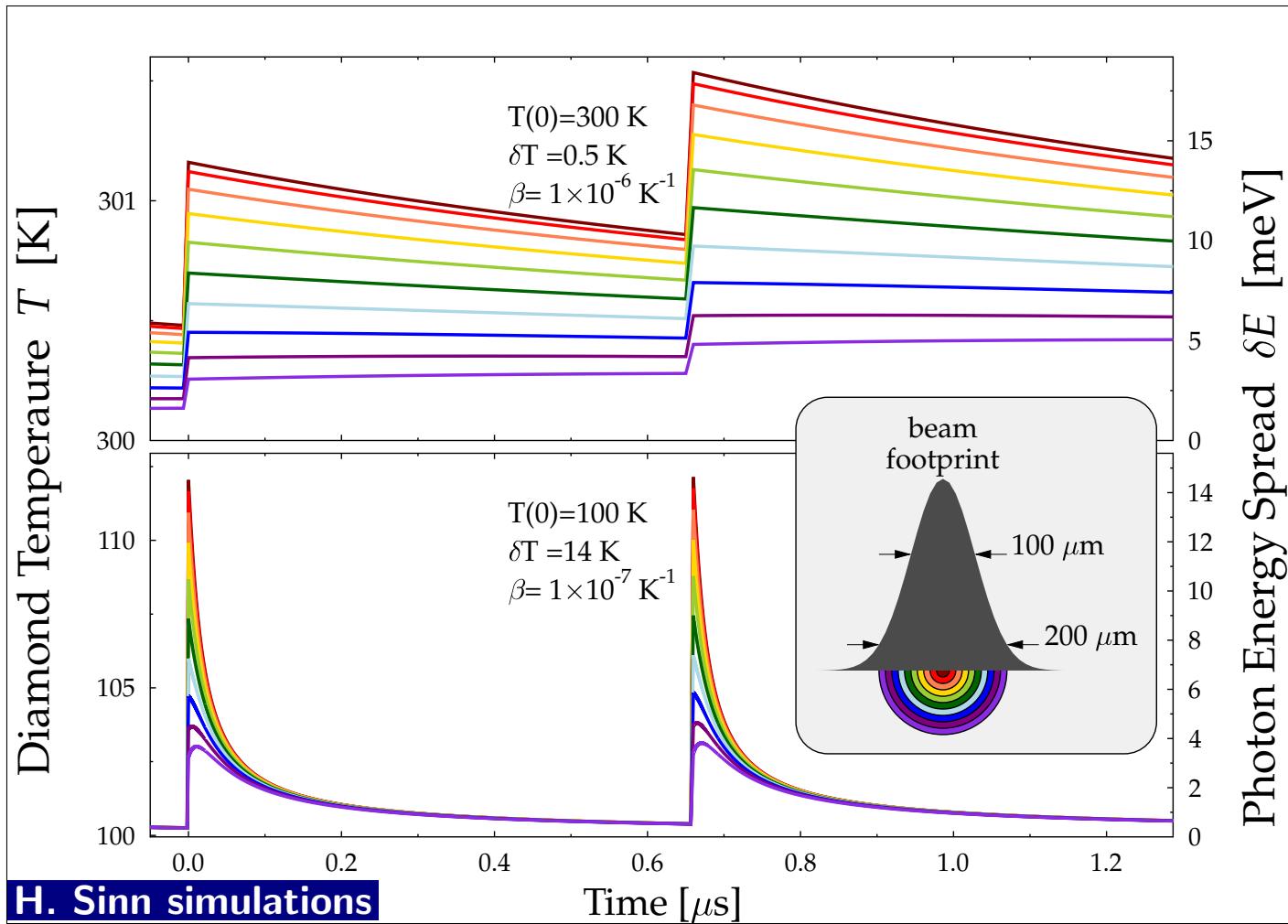
Footprint:  $\simeq 100 \times 100 \mu\text{m}^2$

Is it a problem?

# Heat Load Problem

Temperature gradient  $\delta T \Rightarrow$  energy spread  $\delta E/E = \beta\delta T$ .

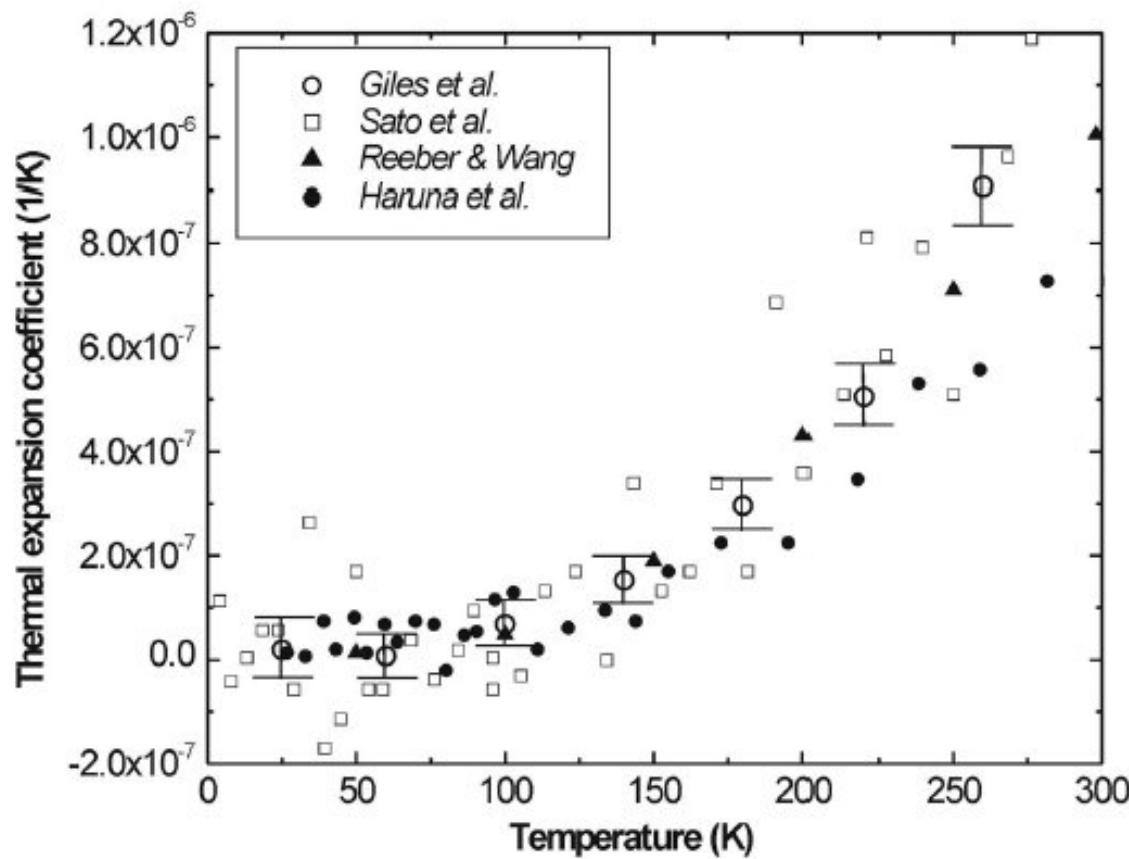
Requirement:  $\delta E \lesssim 1$  meV, when the next pulse arrives.



- Big temperature jump  $\delta T$  after the x-ray pulse arrival.
- $T=300$ K: Big temperature spread by the arrival of the next x-ray pulse.
- $T=100$ K: Negligible temperature spread by the arrival of the next x-ray pulse.
- Reasons:
  1. High temperature diffusivity  $\mathcal{D}$
  2. Low temperature expansion  $\beta$

Solution: Maintain diamond at  $T < 100$  K!

# Thermal Expansion in Diamond < 2009

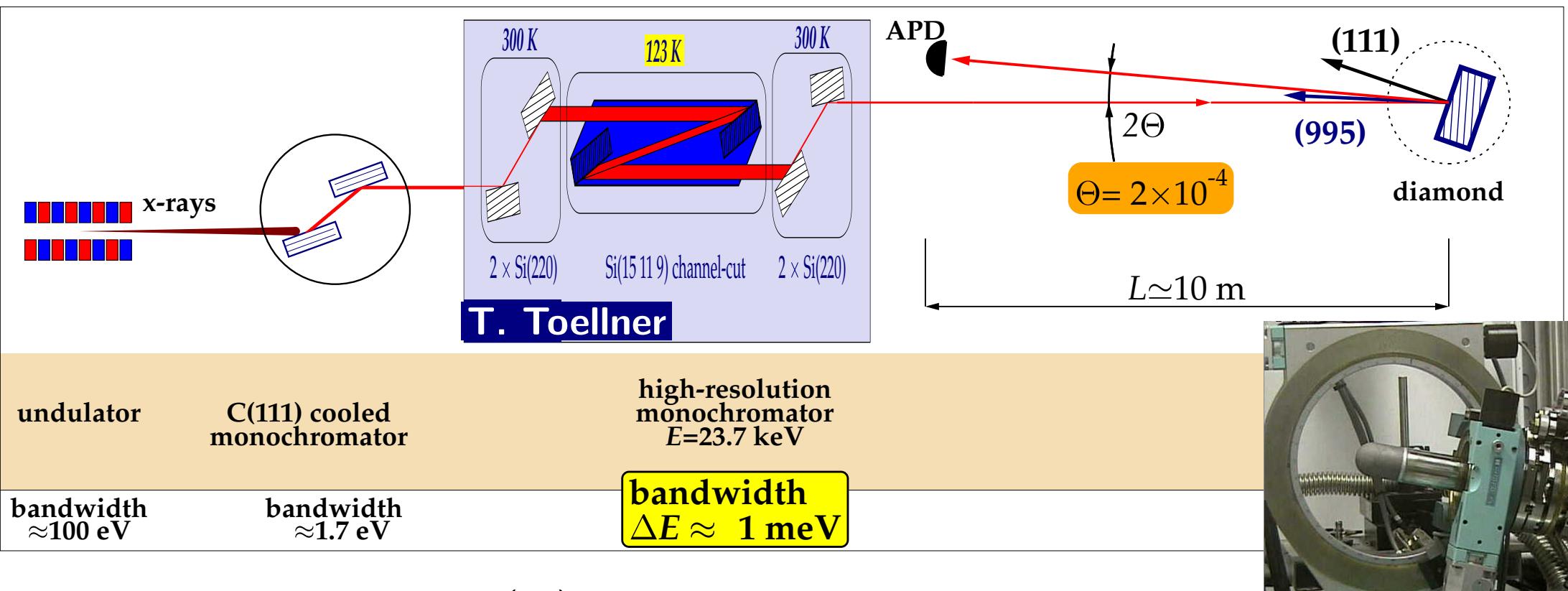


**Figure 5**

Linear thermal expansion coefficient ( $\alpha$ ) obtained in the present work compared with other results found in the recent literature. Values for  $\alpha$  between 30 K and 90 K are of the order of  $1 \times 10^{-7}$ , compatible with published results.

C. Giles et al, J. Synchrotron Rad. (2005). 12, 349

# Diamond Thermal Expansion: Sector 30 @ APS



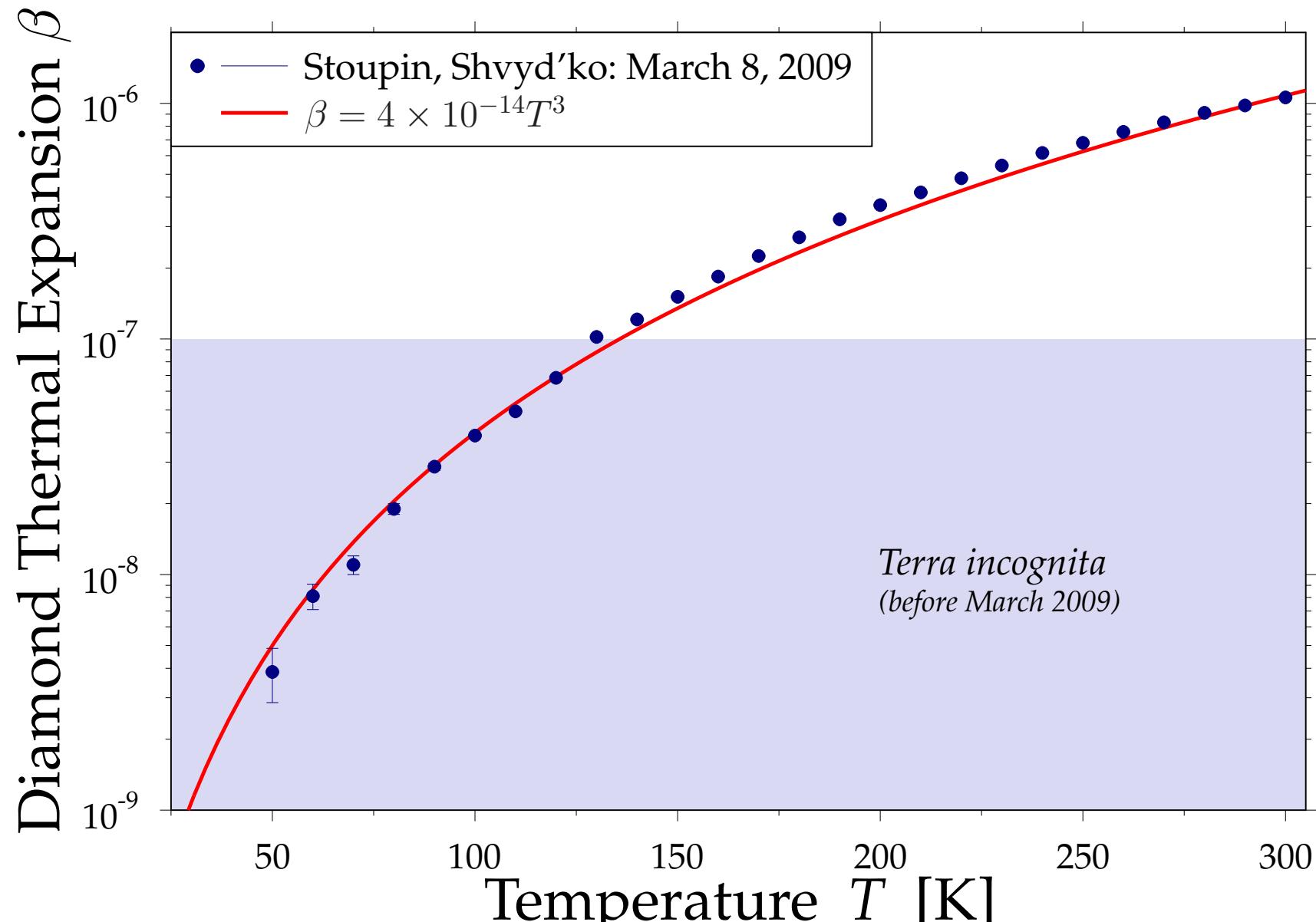
**Bragg's law:**  $\lambda = 2d(T) \sin \theta$

$\theta = \pi/2 - \Theta$  ... in backscattering:  $\lambda = 2d(1 - \Theta^2/2)$

$E = E_H(T)(1 + \Theta^2/2)$ ,  $E_H(T) = hc/2d(T)$

**Uncertainty:**  $\delta E/E_H = \Theta \delta \Theta \ll 10^{-8} \Rightarrow \delta E \ll 0.1$  meV

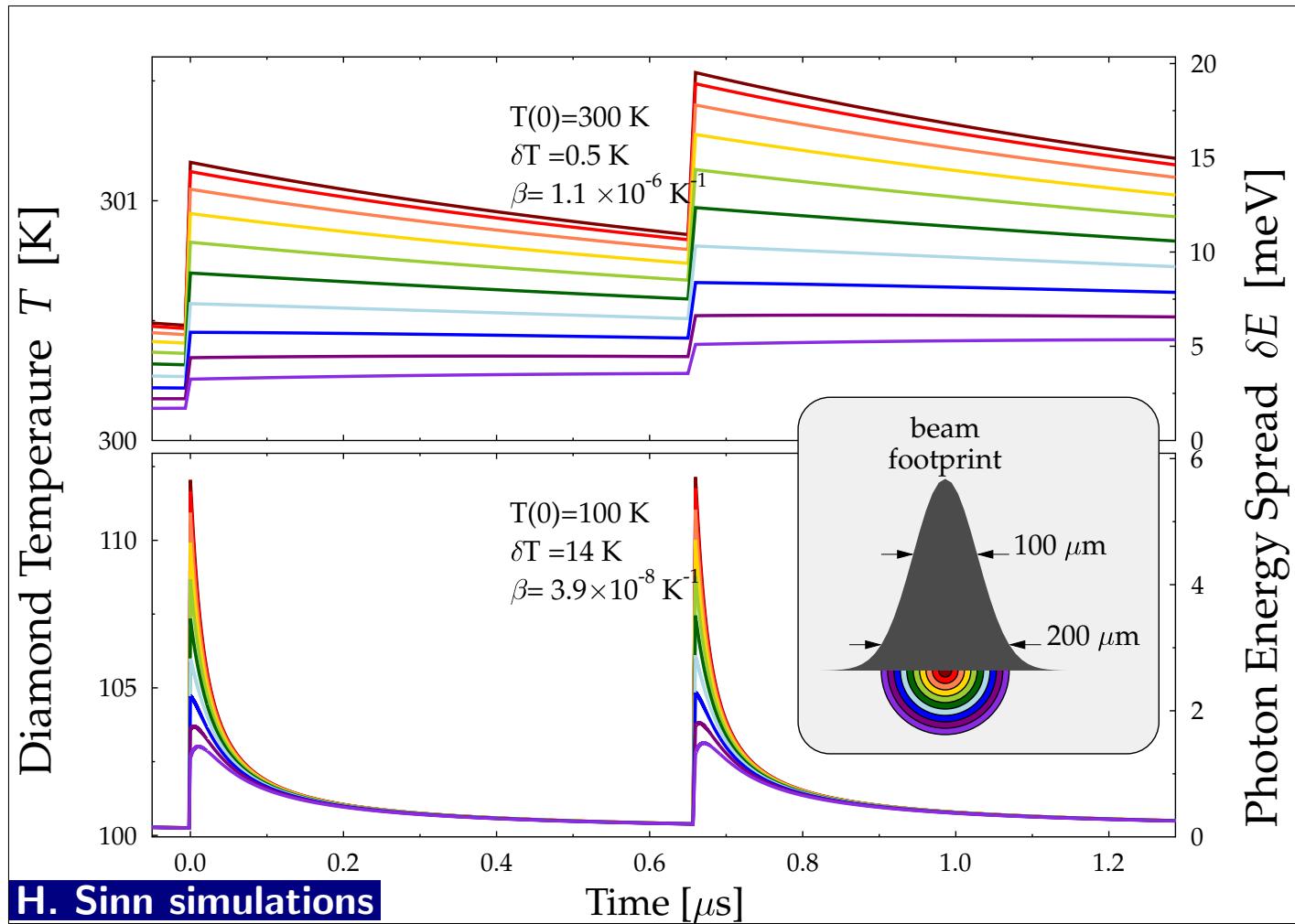
# Diamond Thermal Expansion: APS Sector 30



# Heat Load Problem

Temperature gradient  $\delta T \Rightarrow$  energy spread  $\delta E/E = \beta\delta T$ .

Requirement:  $\delta E \lesssim 1$  meV, when the next pulse arrives.



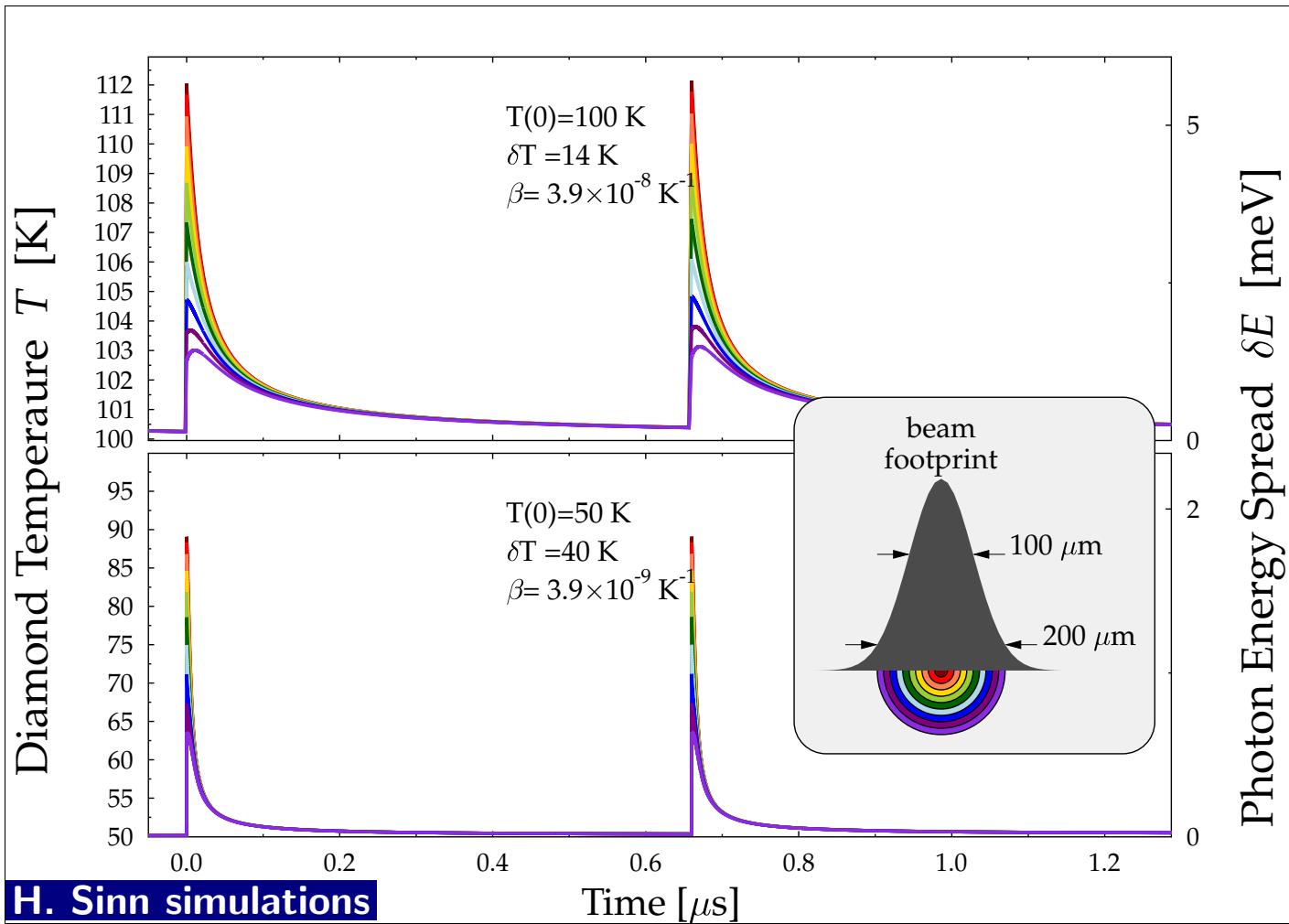
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# Best Temperature for Diamond

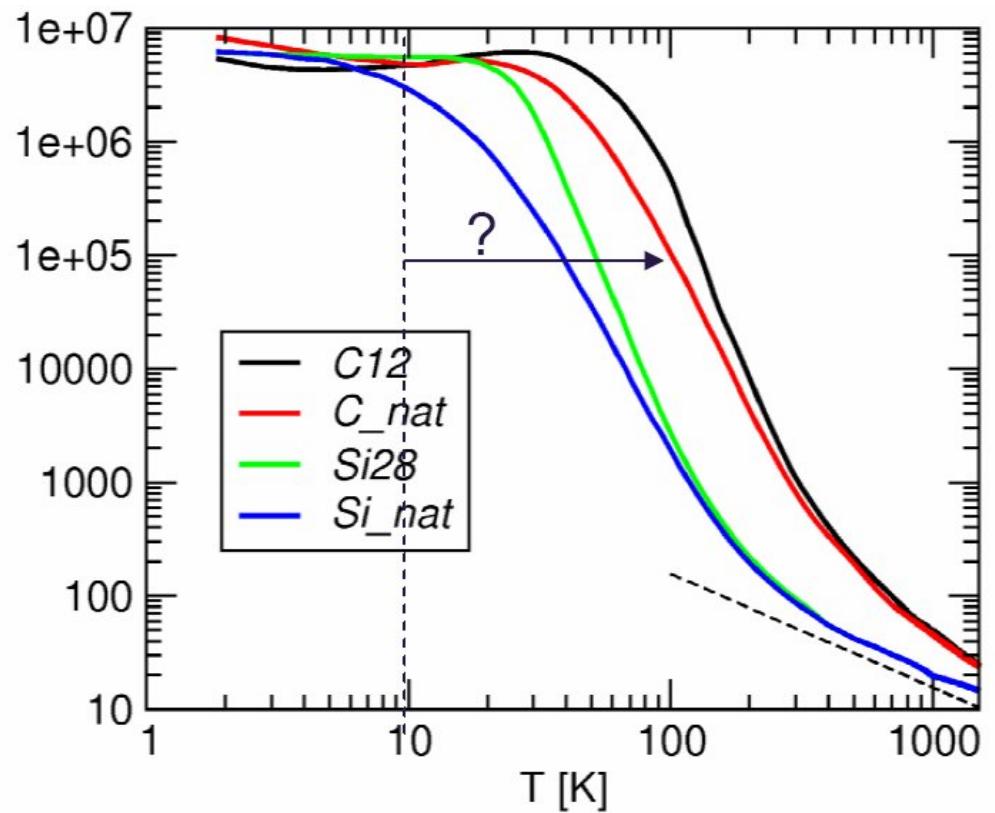
$$\delta E/E \propto \beta(T) \delta T$$

$$\delta T \propto 1/C_v(T) \propto T^{-3}$$

$$\beta \propto C_v \propto T^3$$

$$\delta E/E \simeq \text{const}$$

Best temperature is defined by  
maximum thermal diffusivity

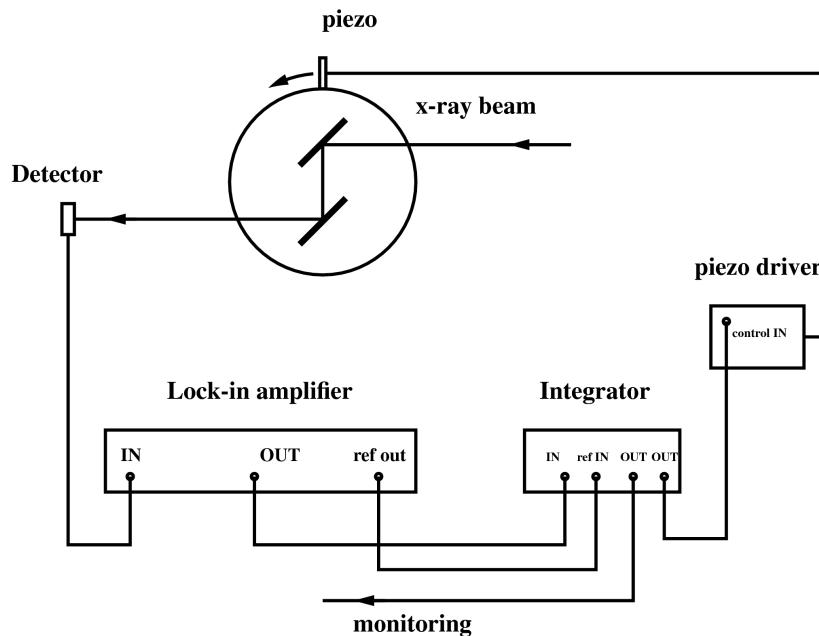
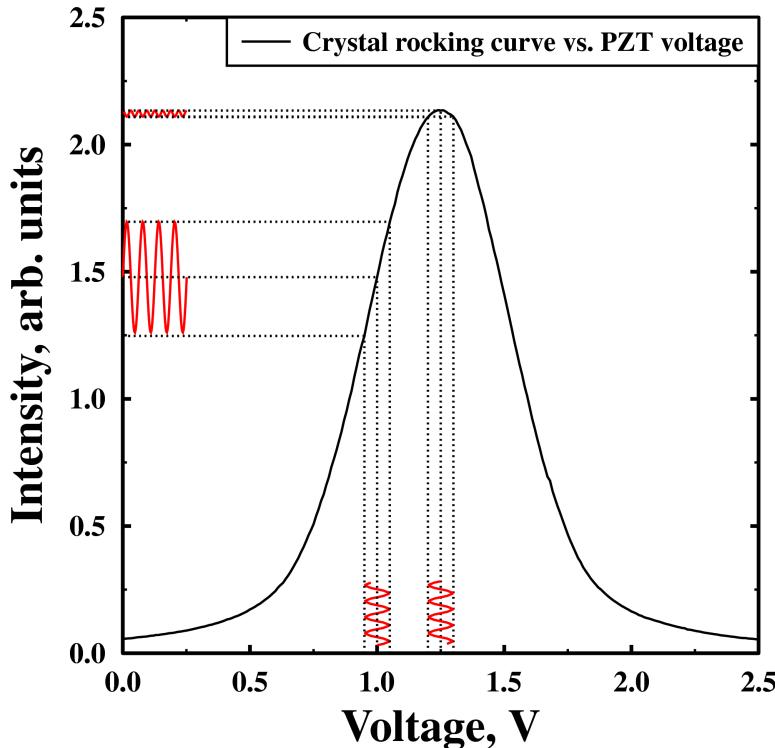


# Angular & Spatial Stability

Required angular stability:  $\delta\theta \lesssim 10 \text{ nrad}$

Required spatial stability:  $\delta L \lesssim 3 \mu\text{m} (\text{rms}) \Rightarrow \delta L/L \simeq 3 \times 10^{-8}$  ( $L = 100 \text{ m}$ )

## Solution: Null-detection hardware feedback. (LIGO prototype)

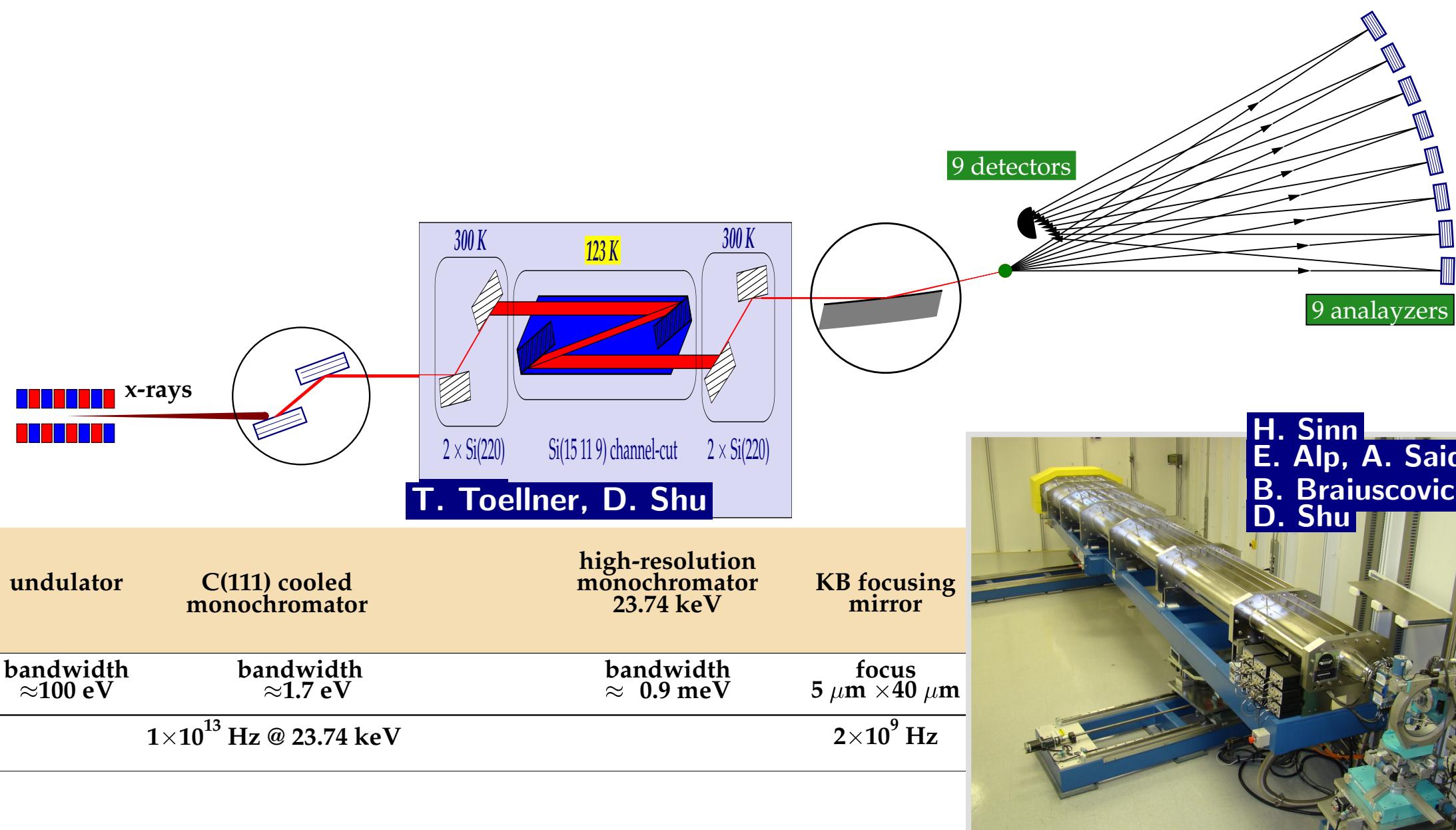


$\simeq 50 \text{ nrad}$  stability was demonstrated at Sector 30

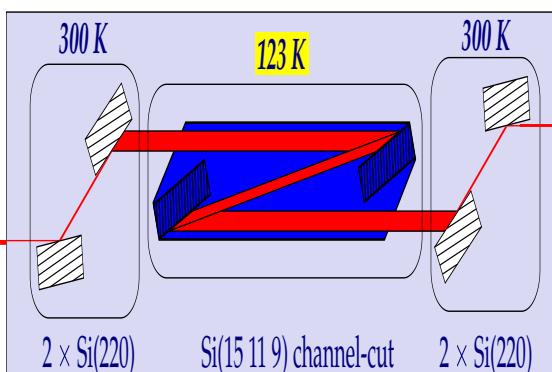
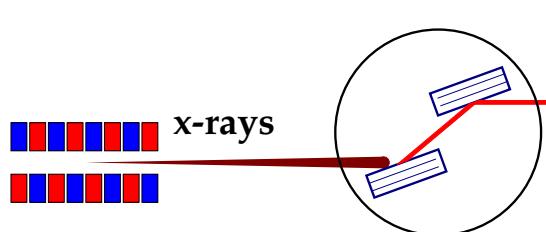
S. Stoupin, F. Lenkszus, R. Laird, K.-J. Kim, Yu. Shvyd'ko

- Transmitted x-ray intensity: the linear response to a small oscillating signal is proportional to angular deviation from the maximum of the rocking curve
- Feedback/correction signal is extracted using lock-in amplification

# HERIX Instrument - Sector 30 @ APS



# HERIX Monochromator



T. Toellner, D. Shu

undulator

C(111) cooled  
monochromator

high-resolution  
monochromator  
23.74 keV

KB focusing  
mirror

bandwidth  
 $\approx 100$  eV

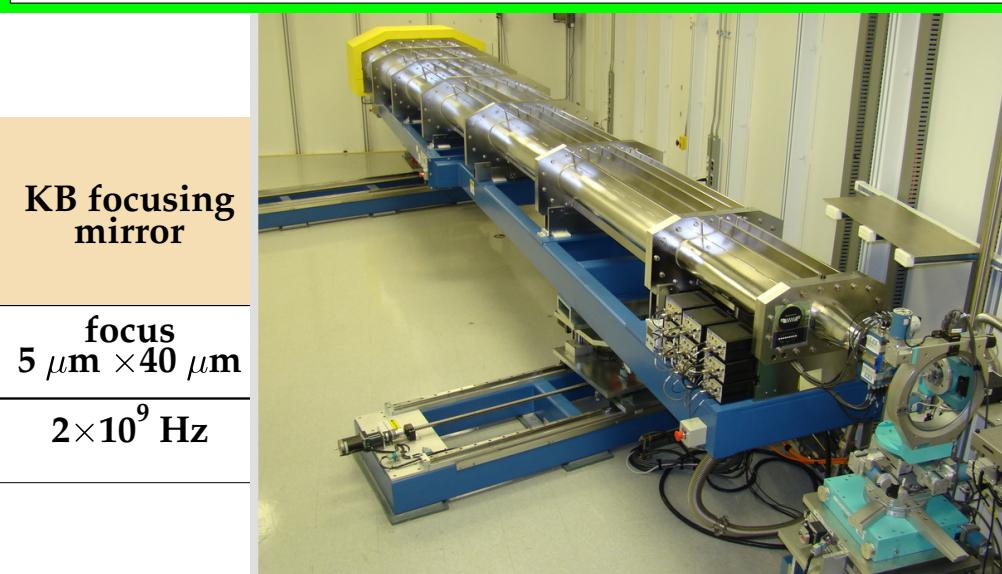
bandwidth  
 $\approx 1.7$  eV

bandwidth  
 $\approx 0.9$  meV

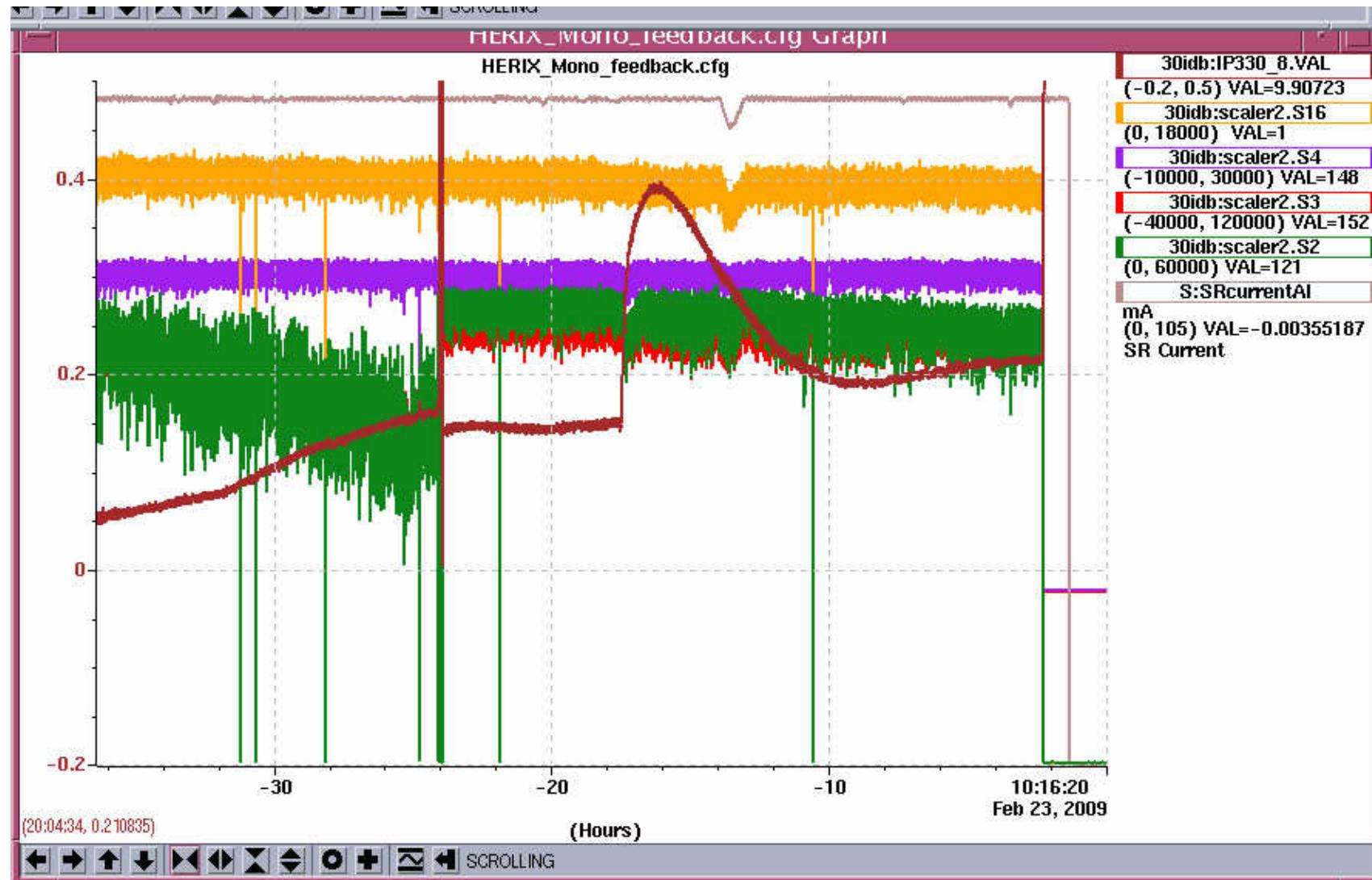
focus  
 $5 \mu\text{m} \times 40 \mu\text{m}$

$1 \times 10^{13}$  Hz @ 23.74 keV

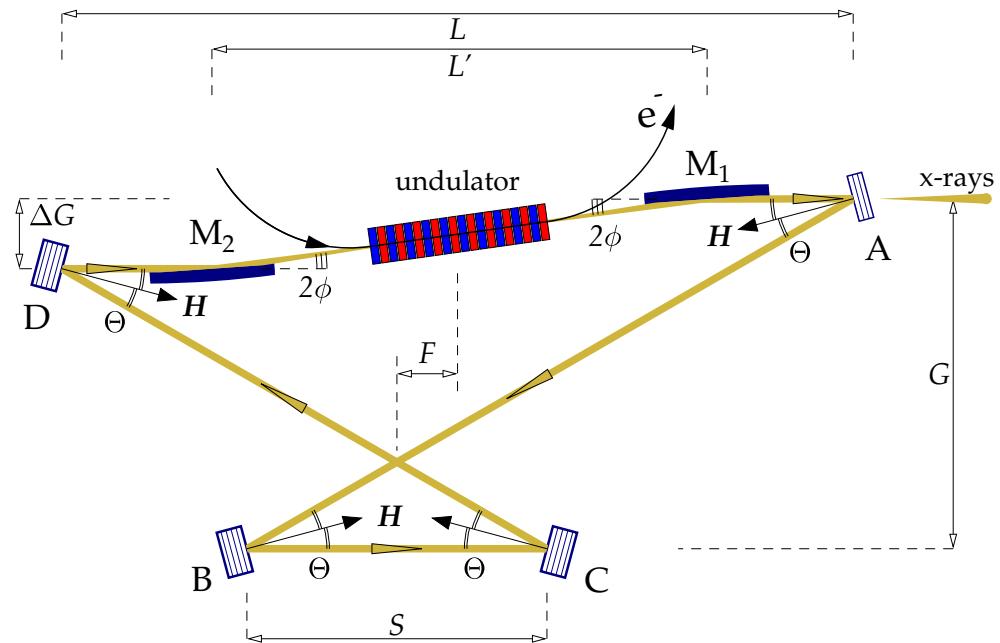
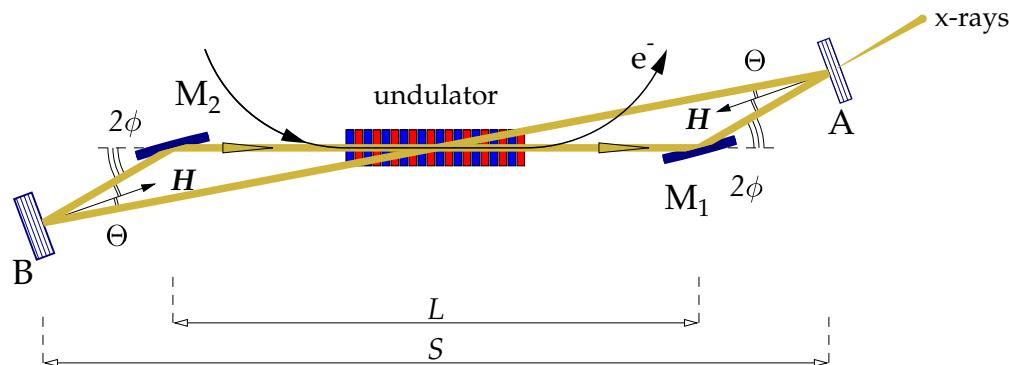
$2 \times 10^9$  Hz



# HERIX Monochromator Stability



# XFELO Technical Challenges



## X-ray Optics:

- Quality of diamond crystals:  
is the theoretical reflectivity achievable? **m. p. yes**
- Heat load problem (reflection region variations  $\lesssim 1 \text{ meV}$ ). **m. p. yes**
- Angular stability:  $\delta\theta \lesssim 10 \text{ nrad}$  **m. p. yes**  
Spatial stability:  $\delta L \lesssim 3 \mu\text{m} (\text{rms}) \rightarrow \delta L/L \lesssim 3 \times 10^{-8}$

# Summary & Outlook

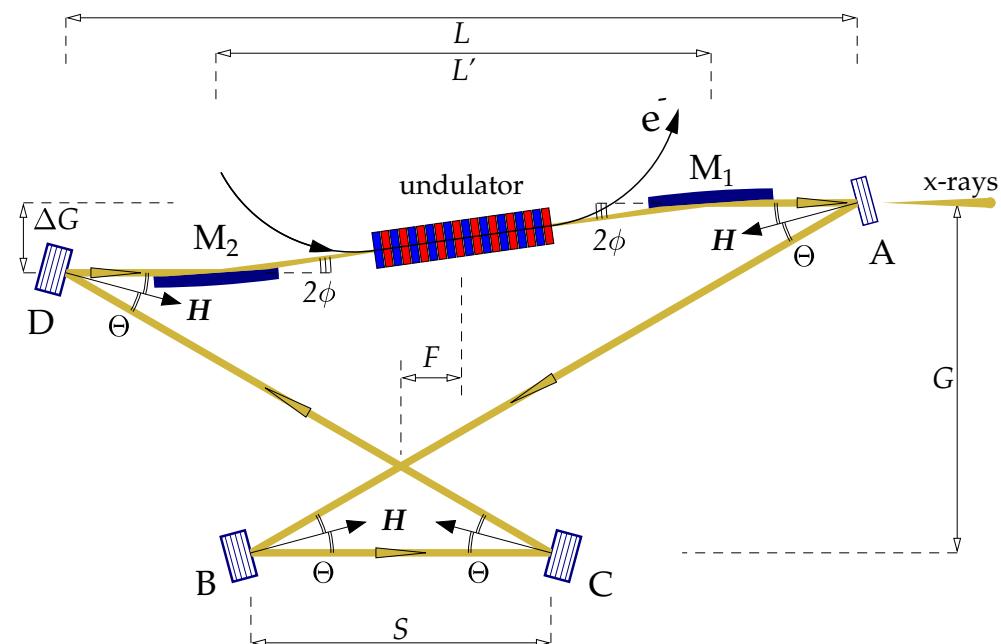
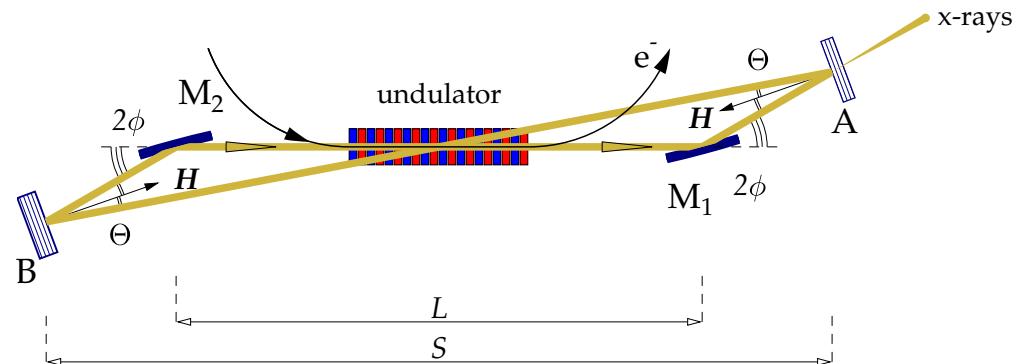
## XFEL-O:

- High set spectral brightness.
- Small energy bandwidth.
- Full coherence. • ps-pulses.

## Applications:

- Nuclear resonant spectroscopies.
- Inelastic X-ray scattering.
- HAXPES. • ps-Time measurements.
- Imaging at near-atomic resolution ( $\simeq 1 \text{ nm}$ ).

Low loss x-ray cavities are feasible! X-ray cavities of different types for the XFEL-O under consideration, including tunable ones.



XFEL-O R+D project is in progress at the APS.

# Acknowledgments

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**Robert Winarski (APS)**

**Tim Gruber (APS)**

**Frank Lenkszus (APS)**

**Robert Laird (APS)**

**Stan Whitcomb (LIGO)**

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**AI Macrander (APS)**

**Lahsen Assoufid (APS)**

**Tom Toellner (APS)**

**Deming Shu (APS)**

**Sven Reiche (UCLA)**

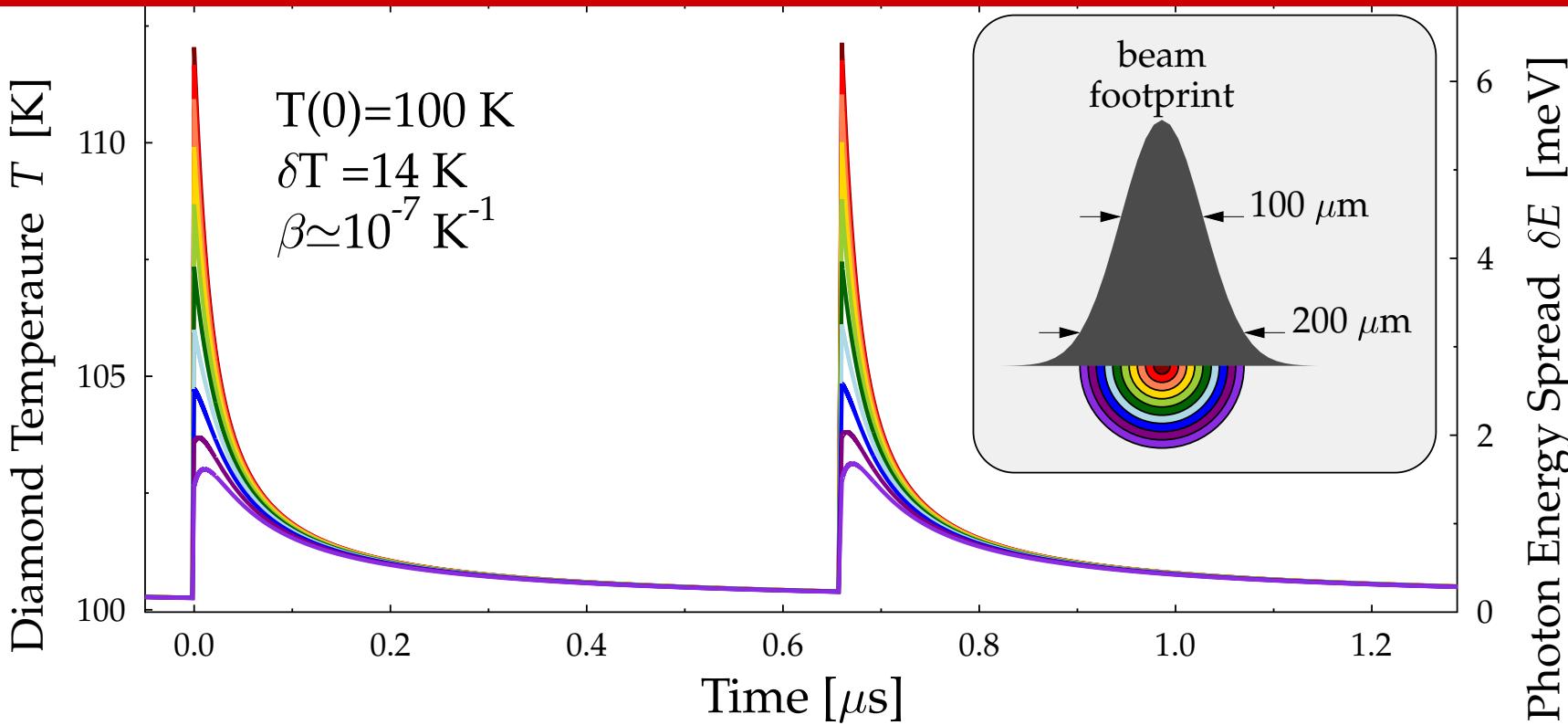
**W. Falley (BNL)**

**Ayman Said (APS)**

**Tim Roberts (APS)**

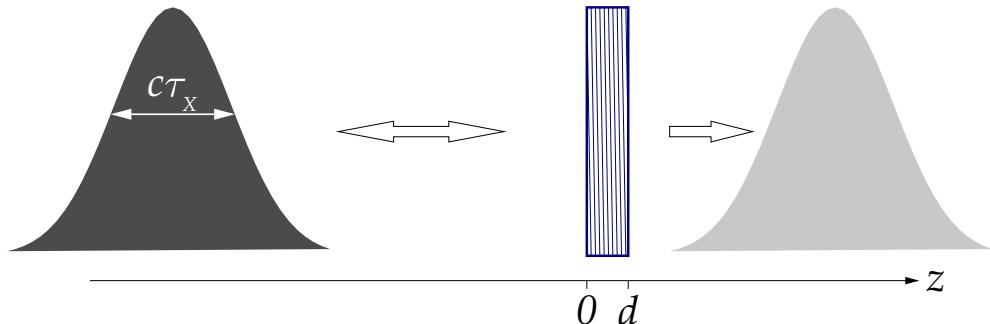
**Emil Trakhtenberg (APS)**

# Heat Shock Waves



How fast the temperature jump  $\delta T$  results in thermal expansion and

in energy variation  $\delta E$ ?

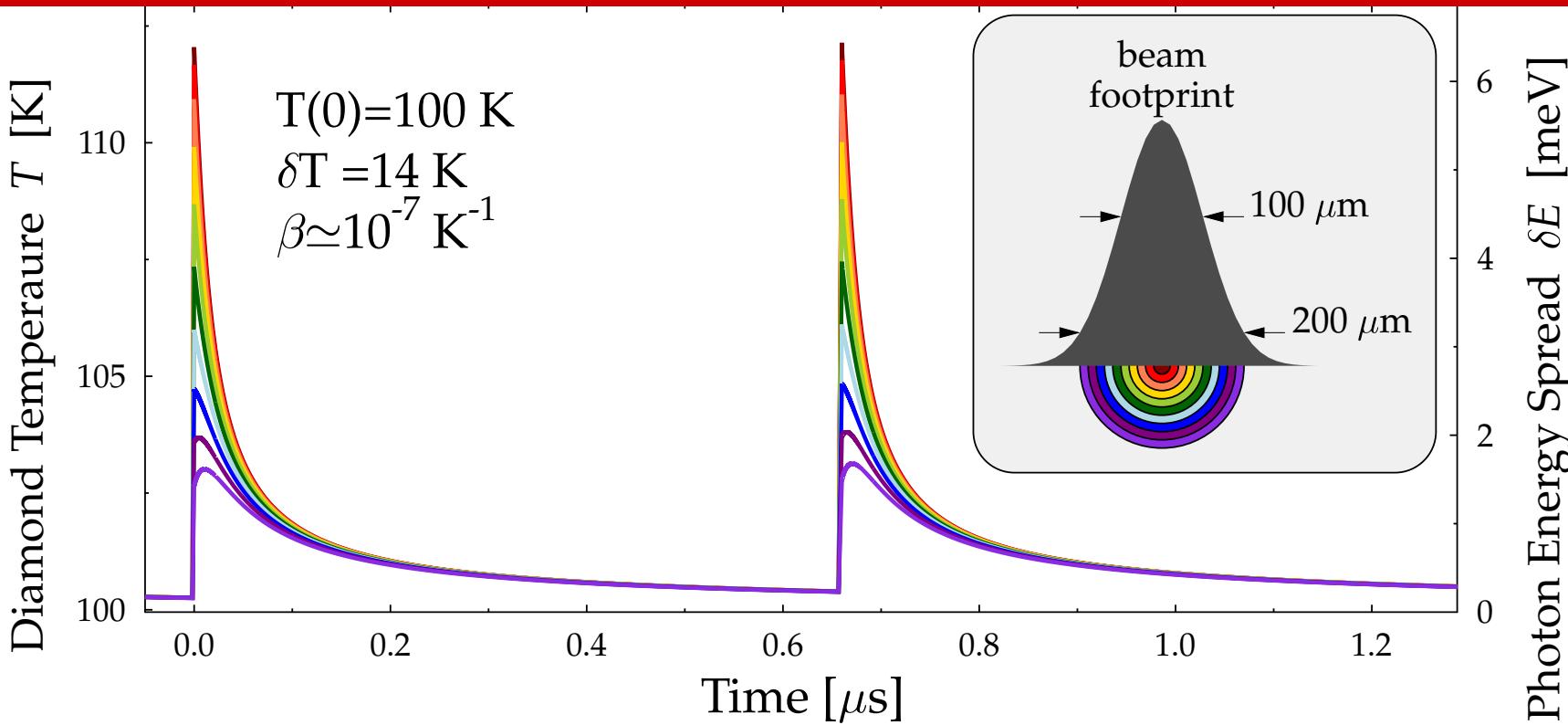


$$\tau_x = 1 \text{ ps (rms)} \Rightarrow c\tau_x = 300 \mu\text{m}$$

$$d \simeq 50 \mu\text{m}$$

Interaction time:  $\tau_x = 1 \text{ ps (rms)}$

# Heat Shock Waves



How fast the temperature jump  $\delta T$  results in thermal expansion and  
in energy variation  $\delta E$ ?

Pedestrian:  $\tau_D = \frac{d}{c_\ell} \simeq 2 \text{ ns}$  [sound velocity  $c_\ell = 1.8 \times 10^4 \text{ km/s}$ ]

Y.C.Lee:  $\tau_D^* = \tau_D \frac{1}{\beta \Delta T} \simeq 1 \text{ ms}$  [J. Phys.: Cond. Matter: 20 (2008) 055202]

Thermal expansion is yet negligible while the pulse is on  $\tau_x \ll \tau_D \ll \tau_D^*$  !!!!