~~Phonons~~ with XPCS

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European XFEL

H. Sinn, User Meeting 2007: Phonon intensity per speckle and pulse

E [keV]	h k l	θ_b	h [mm]	θ_{max} [deg]	Q_{max} [Å^{-1}]	s [μm]	solid angle /speckle [rad^2]	ΔQ /speckle [nm^{-2}]	phts /sec sample	phts /pulse sample	phts /sec total detector [kHz]	phts /pulse total detector	phts /pulse one pixel
12.913	8/8/0	90.0	3.8	5.47	1.25	19	3.6E-12	1.5E-8	2.8 E13	9 E8	**1.0**	0.04	**1.4E-7**
12.913	8/0/0	45.0	3.8	4.11	0.94	19	3.6E-12	1.5E-8	1.2E14	4.1E9	**4.6**	0.15	**6.1E-7**
10.209	8/4/0	90											**4.0E-7**
10.209	6/2/0	45.0											**1.3E-6**
7.908	4/4/4	90.0											**1.0E-6**
7.908	4/2/2	45.0											**3.0E-6**
6.456	4/4/0	90.0	0.53	5.57	0.64	38	1.4E-11	1.5E-8	3.9E14	1.3E10	**15**	0.5	**2.0E-6**
6.456	4/0/0	45.0	0.53	3.43	0.39	38	1.4E-11	1.5E-8	1.0E15	3.4E10	**38**	1.2	**5.1E-6**
4.565	4/0/0	90.0	0.18	7.16	0.57	54	2.9E-11	1.5E-8	1.0E15	3.3E10	**38**	1.2	**5.0E-6**
4.565	2/2/0	45.0	0.18	4.58	0.37	54	2.9E-11	1.5E-8	2.4E15	8.0E10	**90**	3.0	**1.2E-5**

More feasible for THz phonons in crystals:
Pump-probe meV-IXS or
reciprocal lattice mapping

Sample: C of thickness h, Bragg delay line using Si-hkl reflections, 50 micron focus

Outline

Can we observe ‘atomic’ X-ray speckles + higher order correlations from liquids?

If yes, what X-ray optics do we need?

Why could it be feasible?

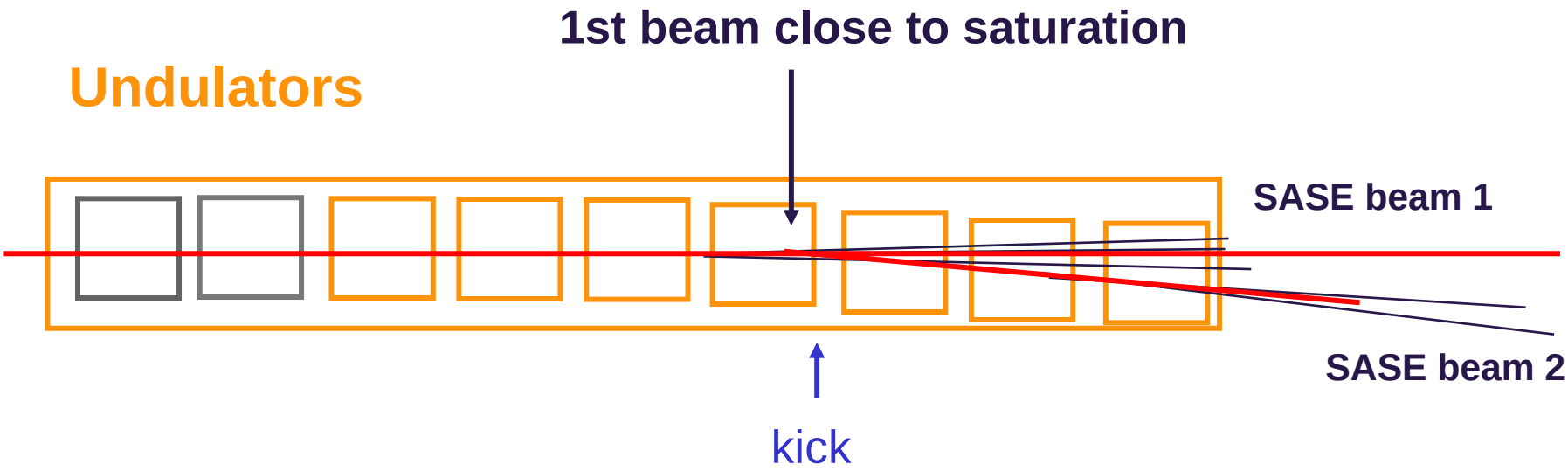
- Experiment Peter Wochner et al. on PMMA spheres:

  1.) Measurement around $S(Q_{max})$
  (more intense than phonons)

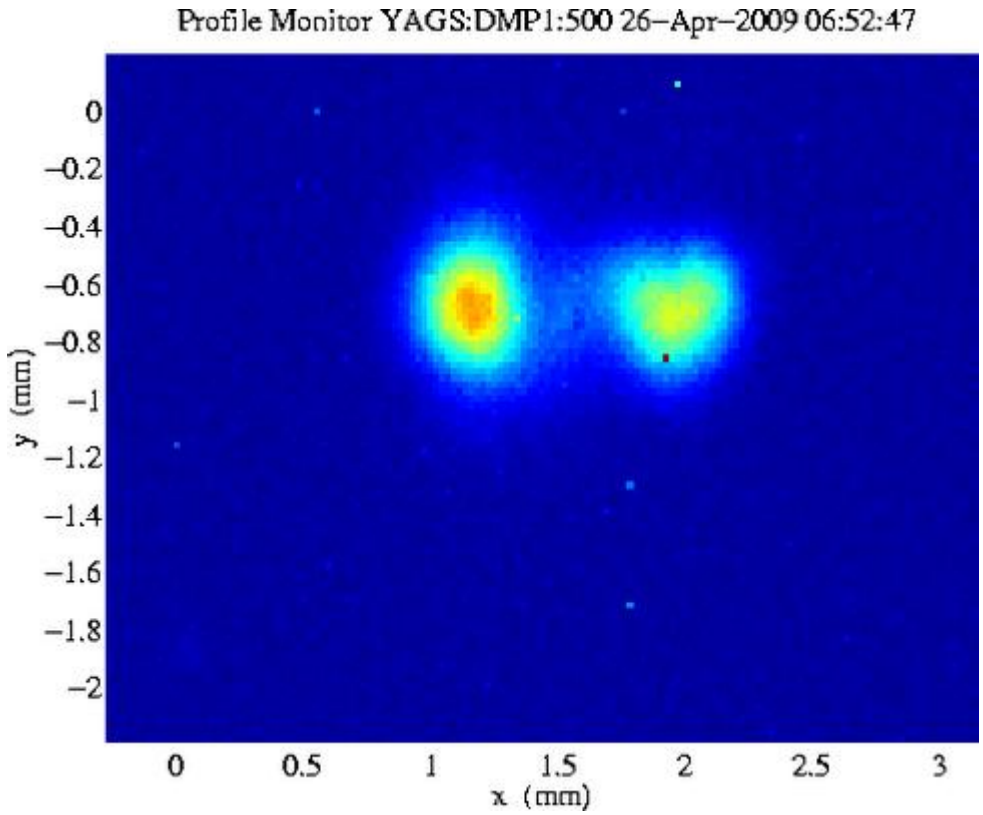
  2.) Static Image (XFEL one shot) reveals already very interesting higher order correlation effects

- More efficient split or delay maybe feasible in accelerator?

Splitting of SASE beam at LCLS

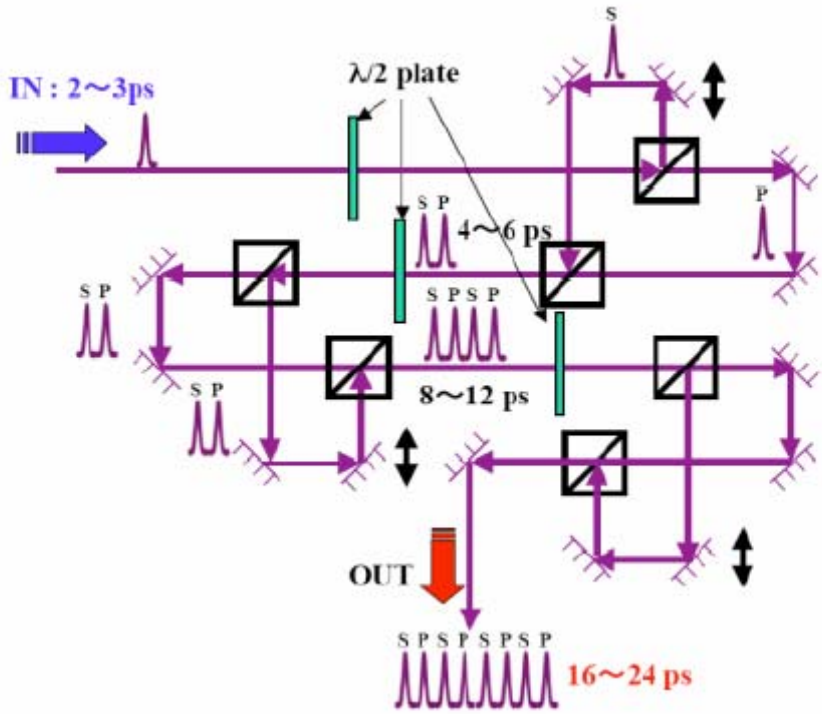


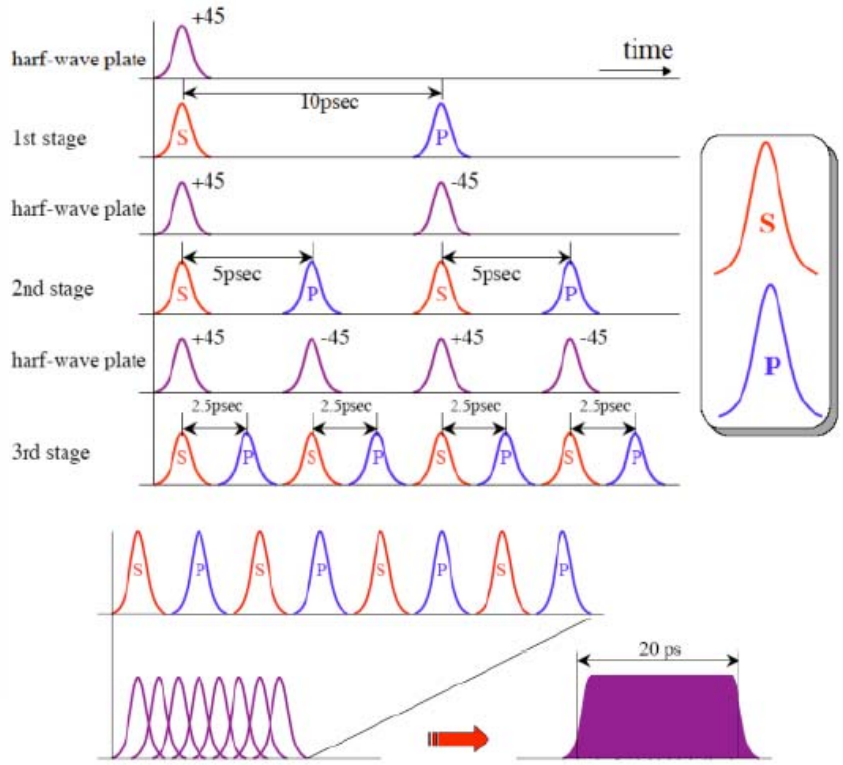
Two FELs next to each other!



F.J. Decker, H.D. Nuhn et al., LCLS April 2009

Split and Delay at RF Gun possible?





H. Dewa et al. Proc. FEL 2006

Delay by one RF cycle would (probably) give two XFEL pulses!

Fundametal RF frequencies: XFEL 1.3 GHz → 770 ps

LCLS 2.8 GHz → 350 ps

Back to speckles:

Is (single shot) speckle pattern from e.g. water observable?

Can we observe speckles on water?

Brian Stephenson's talk and 'LCLS The first experiments, 2003'

$$N_{\min}^{SP} = N_{\min} \frac{\lambda^2}{A} \frac{M_{corr}\sigma_{el}}{2\pi\sigma_{abs}} r_0^2 f^2(Q_{\max}) S(Q_{\max}) \frac{l_{abs}\rho_m}{m_{at}}$$

counts per speckle (min≈1/100)

counts on sample

solid angle per speckle

estimate cross section for atomic liquids

Q_{max}= 2 .. 3 Å^{-1}, $S(Q_{max})$ = 1.5 (water) … 3 (simple liquids)

Can we observe speckles on water?

required intensity per pulse

The smaller the focus the less intensity is needed
(but also N_{min}/A is constant!)

$$N_{\min} = N_{\min}^{SP} \frac{A}{\lambda^2} \frac{m_{at}}{r_0^2 f^2(Q_{\max}) S(Q_{\max}) l_{abs} \rho_m}$$

Calculations for various liquids

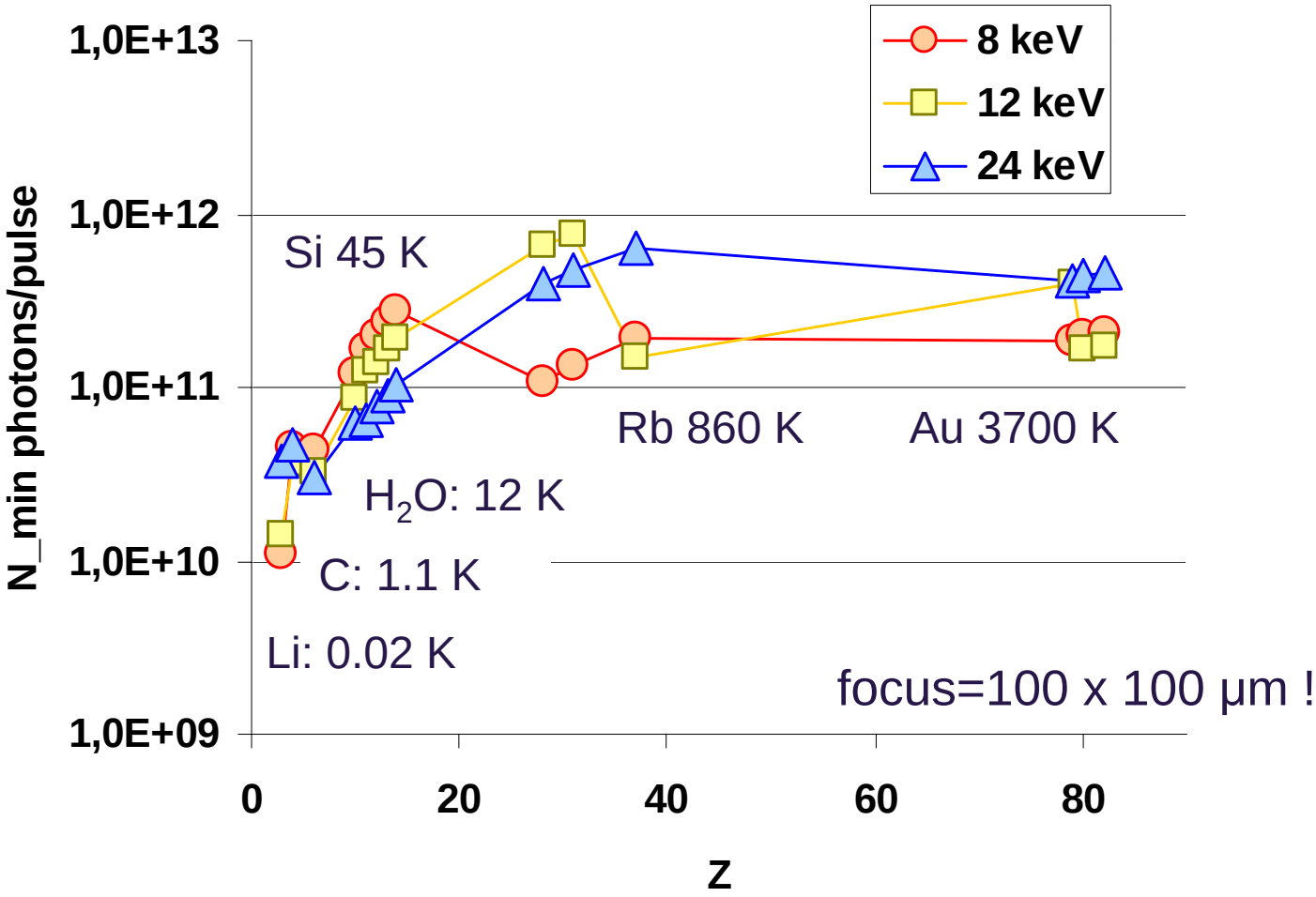
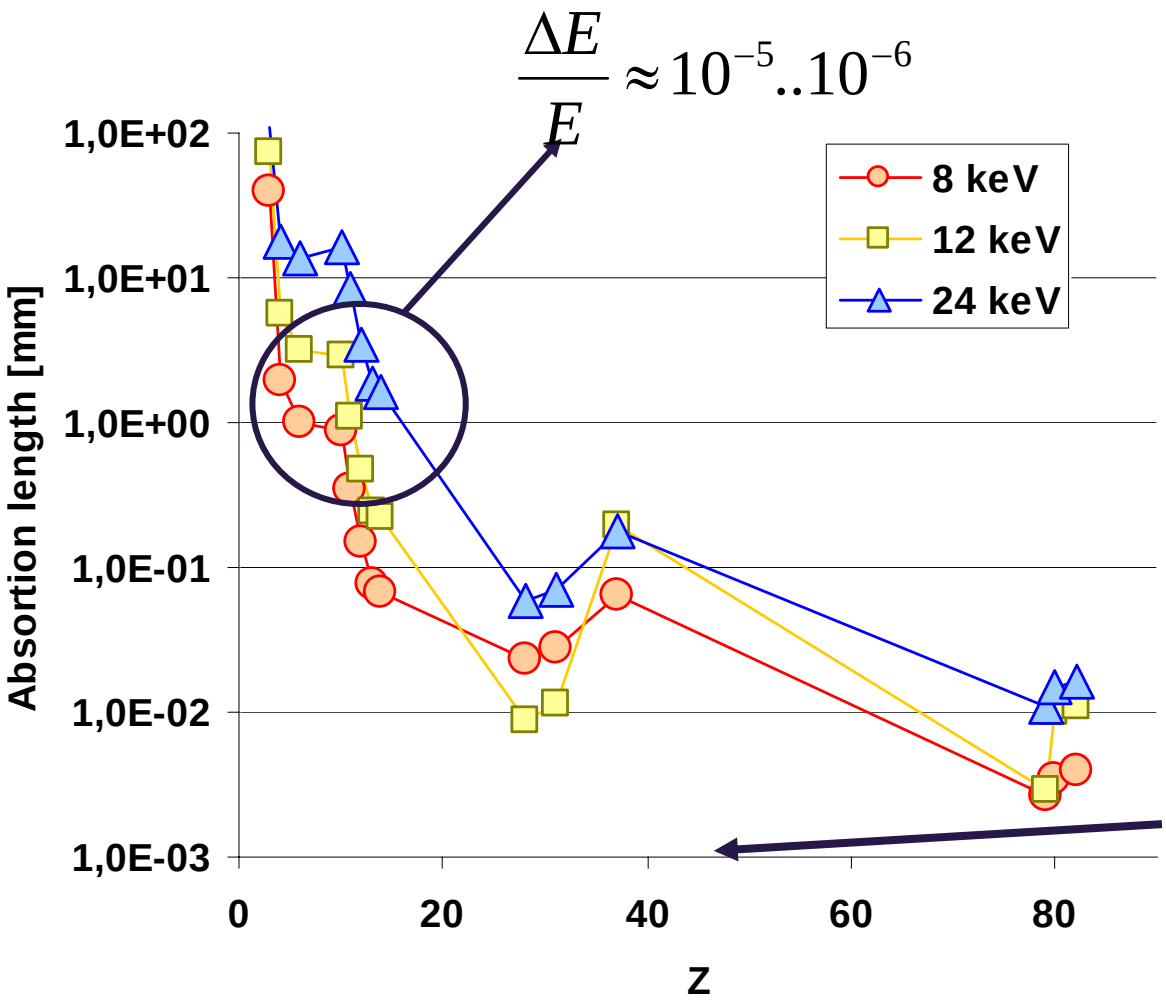


Table for reference

Element	T_m [K]	l_abs 8keV [mm]	l_abs1 2keV	l_abs 24keV	Nmin 8keV	Nmin 12keV	Nmin 24 keV	dT 8keV	dT 12 keV	dT 24 keV
Li	453	39,5000	73,0000	108,0000	1,1E+10	1,4E+10	3,7E+10	0,02	0,02	0,07
B	2365	1,9100	5,6000	17,4000	4,5E+10	3,6E+10	4,6E+10	0,56	0,23	0,19
C	3825	1,0100	3,2000	13,4000	4,4E+10	3,2E+10	3,1E+10	1,18	0,41	0,19
H2O	**273**	**0,8890**	**2,9000**	**16,0000**	**1,2E+11**	**8,6E+10**	**6,3E+10**	**12,64**	**4,13**	**1,08**
Na	371	0,3510	1,1000	8,3000	1,7E+11	1,2E+11	6,6E+10	58,02	20,56	2,88
Mg	922	0,1460	0,4800	3,5000	2,0E+11	1,4E+11	7,7E+10	97,92	31,53	4,74
Al	933	0,0753	0,2470	1,8200	2,4E+11	1,7E+11	9,0E+10	160,59	51,94	7,64
Si	1683	0,0679	0,2210	1,6400	2,7E+11	1,9E+11	1,0E+11	247,70	81,37	11,80
Ni	1726	0,0234	0,0087	0,0585	1,1E+11	6,7E+11	4,0E+11	156,11	3894,31	694,40
Ga	302	0,0277	0,0113	0,0717	1,3E+11	7,6E+11	4,8E+11	290,87	6082,48	1206,88
Rb	312	0,0637	0,1920	0,1780	1,9E+11	1,5E+11	6,4E+11	865,57	331,56	3081,67
Au	1337	0,0026	0,0029	0,0109	1,9E+11	3,9E+11	4,2E+11	3775,27	10715,5	6017,57
Hg	234	0,0035	0,0098	0,0147	2,0E+11	1,6E+11	4,4E+11	4234,99	1900,53	6789,10
Pb	601	0,0039	0,0109	0,0165	2,1E+11	1,7E+11	4,6E+11	4945,58	2237,32	7799,72

But: Absorption length maybe long!



10^3

$$\xi_L = \frac{\lambda}{2} \quad \frac{E}{\Delta E}$$

$$\approx 100\ \text{nm}$$

$$l_{\max} = \xi_L / 2 \sin\theta \tan\theta$$

$$\approx 0.5..1.5\ \mu\text{m}$$

Two possibilities

1. Make water film only 1 micron thick

→ loose factor 900 in scattered intensity

→ use 10^{12} primary intensity and 10x10 micron focus

→ dT = 1200K/shot

2. Increase l_{max} to e.g. 100 μm ($\Delta E/E = 10^{-5}$)

→ loose factor 100 in primary intensity

→ gain factor 100 by using 10 x 10 micron focus

→ dT=12 K/shot

Summary

Beamline Requirements:

for water: dE/E=10^{-5} (100 meV)
focus 10 micron
sample thickness: < 100 micron
beam line efficiency > 10%
dT 12 K → rep rate: slow (jet possible)

higher Z: dE/E=10^{-4} (1 eV)
focus 10 micron
sample thickness: < 10 micron
multiple exposure possible for E → 20 keV

Thank you for your attention!