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Thermal deformation, wavefront distortion, and thermal scattering analysis on cryogenic monochromator

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4th Diffraction Limited Storage Ring (DLSR) Workshop
APS, Argonne National Laboratory.

Nov 20, 2014

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- Characteristics of Cornell ERL undulator radiation
- Modified Linear Power Density (MLPD) and ANSYS simulations
- Wavefront simulation of X-rays through cryogenic mono
- An example of X-ray scattering analysis of cryogenic mono

Cornell ERL source and undulators

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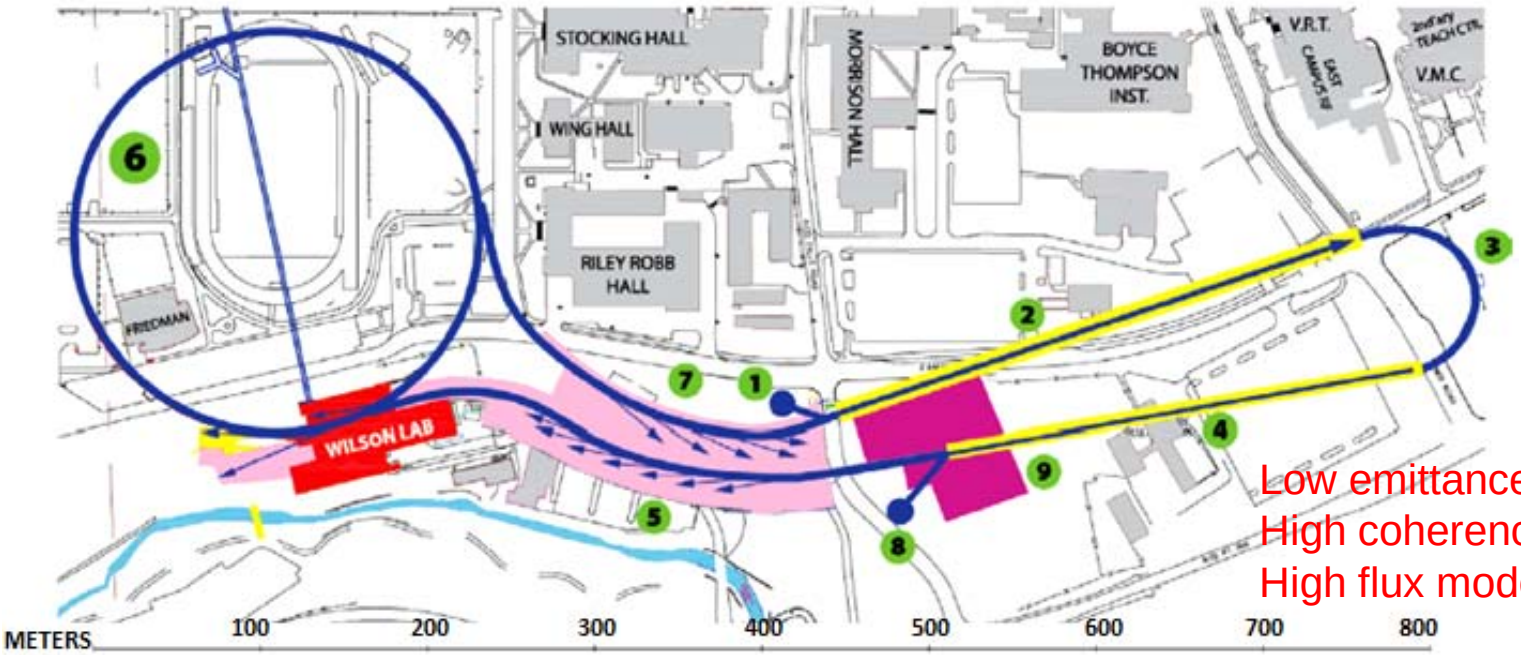
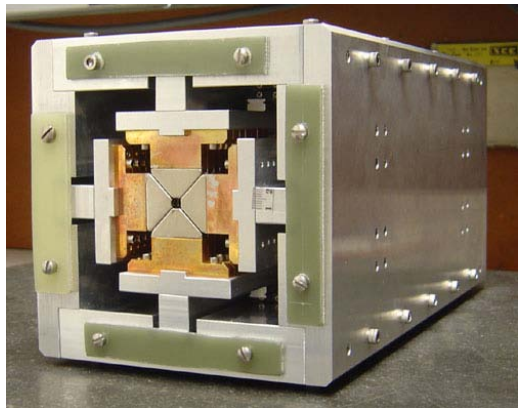


Low emittance & round beam
High coherence mode: 25 mA
High flux mode: 100mA



Delta undulators:
Small gap in both transverse directions;
K tuning by slide magnet array;
Polarizations: planar & helical;
5 m and 25 m long. Period: 19 mm

8 possible combinations of source parameters

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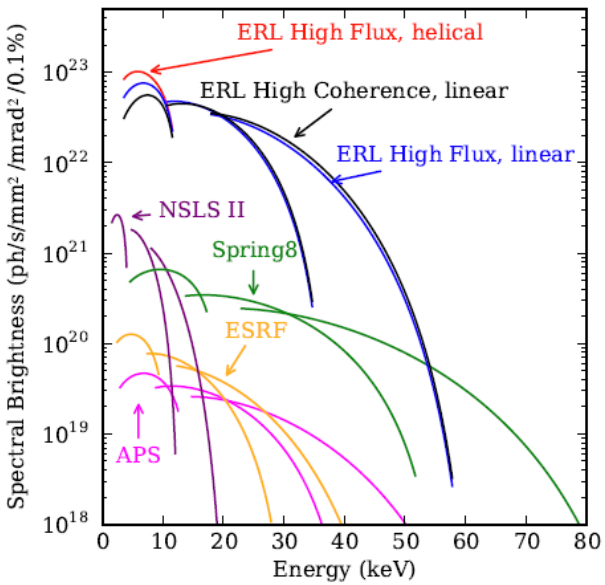
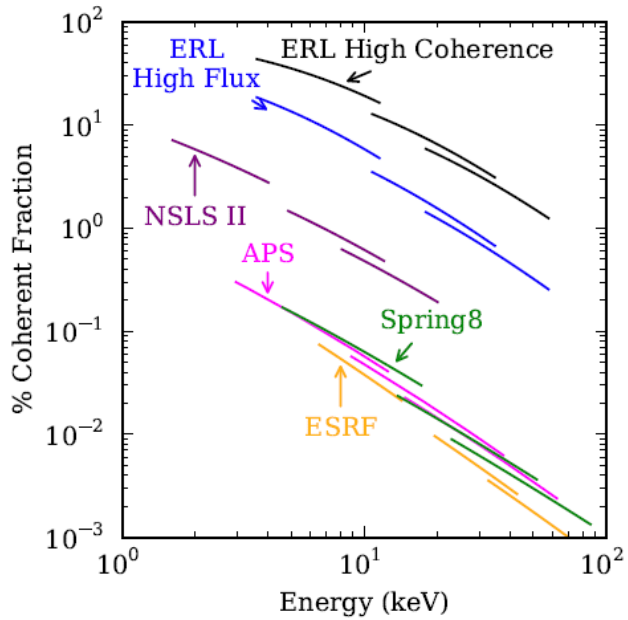
Electron source	High flux 5 m planar	High coherence 5 m planar	High flux 5 m helical	High coherence 5 m helical	High flux 25 m planar	High coherence 25 m planar	High flux 25 m helical	High coherence 25 m helical
$\Delta E/E$ (%)	0.0186	0.0088	0.0186	0.0088	0.0186	0.0088	0.0186	0.0088
Current(mA)	100	25	100	25	100	25	100	25
$\varepsilon_x/\varepsilon_y$ (nm rad)	0.031/0.025	0.013/0.011	0.031/0.025	0.013/0.011	0.031/0.025	0.013/0.011	0.031/0.025	0.013/0.011
β_x/β_y (m)	0.796/0.796	0.796/0.796	0.796/0.796	0.796/0.796	3.98/3.98	3.98/3.98	3.98/3.98	3.98/3.98
σ_x/σ_y (μm)	4.95/4.45	3.217/2.904	4.95/4.45	3.217/2.904	11.1/9.95	7.19/6.49	11.1/9.95	7.19/6.49
σ'_x/σ'_y (μrad)	6.22/5.59	4.042/3.649	6.22/5.59	4.042/3.649	2.78/2.50	1.81/1.63	2.78/2.5	1.81/1.63
Undulator Parameters								
Period number	263	263	263	263	1315	1315	1315	1315
B_{max} (T)	1.2524	1.2524	0.8856	0.8856	1.2524	1.2524	0.8856	0.8856
K_{max}	2.222	2.222	1.57113	1.57113	2.222	2.222	1.57113	1.57113
Beamline parameters @ 8keV								
Σ_x/Σ_y (μm)	5.86/5.44	4.49/4.27	5.86/5.44	4.49/4.27	13.1/12.2	10.0/9.55	13.1/12.2	10.0/9.55
Σ'_x/Σ'_y (μrad)	7.36/6.84	5.64/5.37	7.36/6.84	5.64/5.37	3.29/3.06	2.52/2.40	3.29/3.06	2.52/2.40
Brightness[a]	1.74×10^{22}	1.20×10^{22}	2.13×10^{22}	1.47×10^{22}	8.69×10^{22}	6.00×10^{22}	1.07×10^{23}	7.38×10^{22}
Coherent flux[b]	1.03×10^{14}	7.19×10^{13}	1.27×10^{14}	8.83×10^{13}	4.34×10^{14}	3.32×10^{14}	5.33×10^{14}	4.08×10^{18}
Coherent fraction (%)	9.38	26.1	9.38	26.1	7.88	24.1	7.88	24.1

(a) In unit of ph/s/mm²/mrad²/0.1%B.W. (b) In unit of ph/s/0.1%B.W.

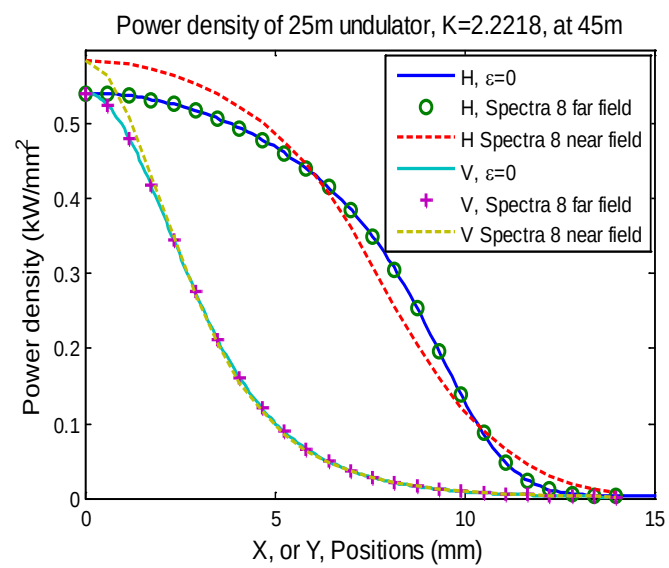
$$\beta = \frac{L}{2\pi} \qquad \sigma_r = \frac{\sqrt{2\lambda L}}{4\pi} \qquad \sigma'_r = \sqrt{\frac{\lambda}{2L}}$$

Characteristics of ERL sources





Cornell ERL: Project Definition Design Report (PDDR)



Radiation power of ERL sources

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On-axis maximum power density of Cornell ERL beamlines under high flux mode.

	ERL planar	ERL planar	ERL helical	ERL helical
N	1315	263	1315	263
L (m)	25	5	25	5
λ_u (m)	0.019	0.019	0.019	0.019
K	2.2218	2.2218	$Kx = Ky = 0.707$	$Kx = Ky = 0.707$
$dP/d\Omega$ (W mrad^{-2})	1.10×10^6	2.18×10^5	3.40×10^5	6.80×10^4

	APS U-A	ESRF ID-27	SPring-8 BL19XU	NSLS-II U20	PETRA III U32 10m	ERL Hi-flux* 25m
N	72	173	780	150	2x156	1315
λ (m)	0.033	0.023	0.032	0.02	0.0314	
E(GeV)	7.0	6.03	8.0	3.0	6	5.0
B_0max (T)	0.891	0.75	0.59	0.97	0.68	1.25
I (A)	0.1	0.2	0.1	0.5	0.1	0.1
dP/dΩ (W/mrad^2)	1.64E5	2.68E5	1.98E6	6.25E4	3.0E5	1.089E6

Length of 12 beamlines

Undulator length (m)	Beamline length (m)	Ratchet wall to source center (m)
5	55	25
5	75	32.5
5	75	32.5
5	75	32.5
25	**85**	**43**
25	**95**	**47**
5	81	30
5	81	30
5	81	30
5	78	30
5	58	24
25	**82**	**37**

Assume mono locations:
35m from source for 5 m undulators
45m from source for 25m undulators

Requirement for mono: tolerate high power density
preserve high quality of beam

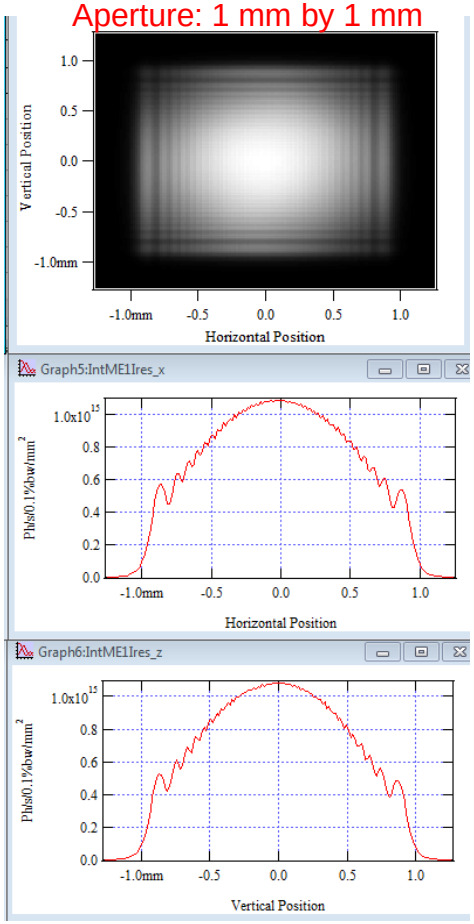
Beam current (mA)	Slit size (H × V) (mm)	Distance to source (m)	Radiation power FWHM (H × V) (mm)	Power in central cone (W)	K
25 m-long planar undulator					
100	0.85 × 0.85	45	16.9 × 5.9	391	2.22
25	0.85 × 0.85	45	16.9 × 5.9	98	2.22
100	0.75 × 0.75	45	8.02 × 5.6	141	1.06
25	0.75 × 0.75	45	8.02 × 5.6	35	1.06
5 m-long planar undulator					
100	1.5 × 1.5	35	13.2 × 4.6	401	2.22
25	1.5 × 1.5	35	13.2 × 4.6	101	2.22
100	1.3 × 1.3	35	6.3 × 4.4	140	1.06
25	1.3 × 1.3	35	6.3 × 4.4	35	1.06
25 m-long helical undulator					
100	0.75 × 0.75	45	8.1 × 8.1	95	0.707
25	0.75 × .75	45	8.1 × 8.1	24	0.707
5 m-long helical undulator					
100	1.3 × 1.3	35	6.3 × 6.3	94	0.707
25	1.3 × 1.3	35	6.3 × 6.3	24	0.707

The power limiting aperture for ERL mono: accept whole central cone

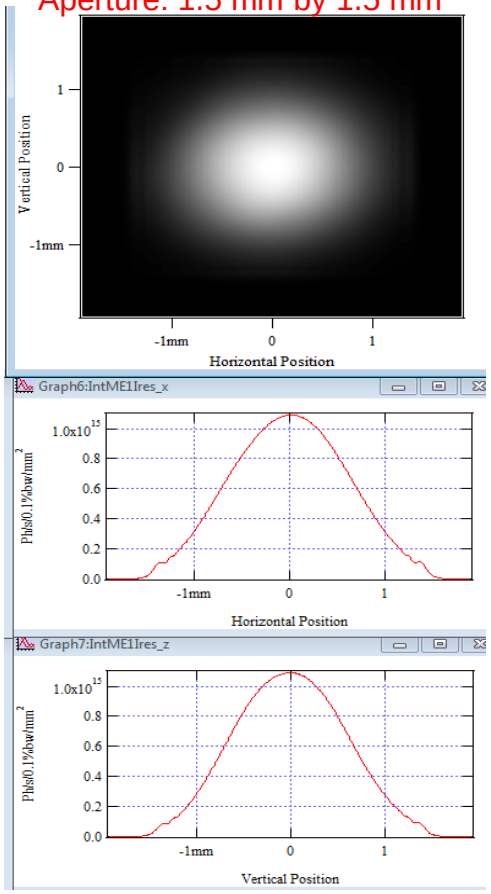
- For 3rd generation source, power aperture can cut into central cone.
- For ERL, accepting whole central cone can avoid fringes at downstream.

5m undulator, high flux mode, 3.6keV, aperture at 35m, X-ray profile at 70m

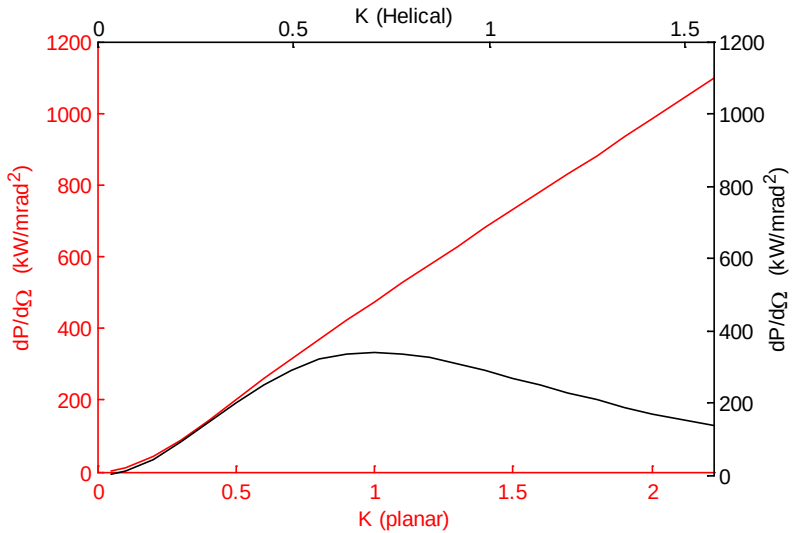
Aperture: 1 mm by 1 mm



Aperture: 1.5 mm by 1.5 mm



- Less on-axis radiation power for undulators in helical mode.



Helical undulator has maximum on-axis power density when K=0.707.

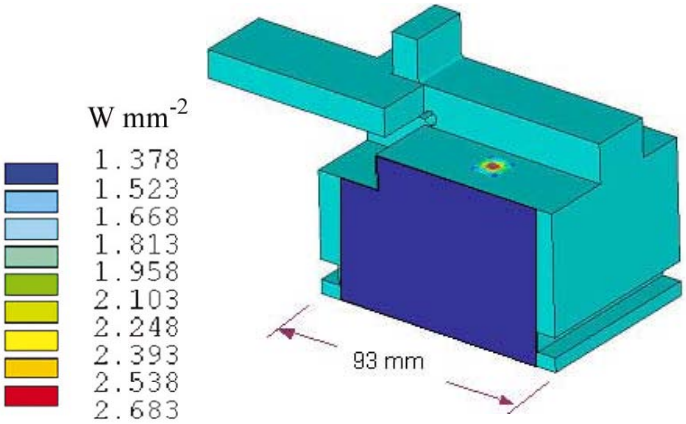
- Radiation power in ERL undulator central cone comparable to 3rd sources, and can be similar for undulators of different lengths.

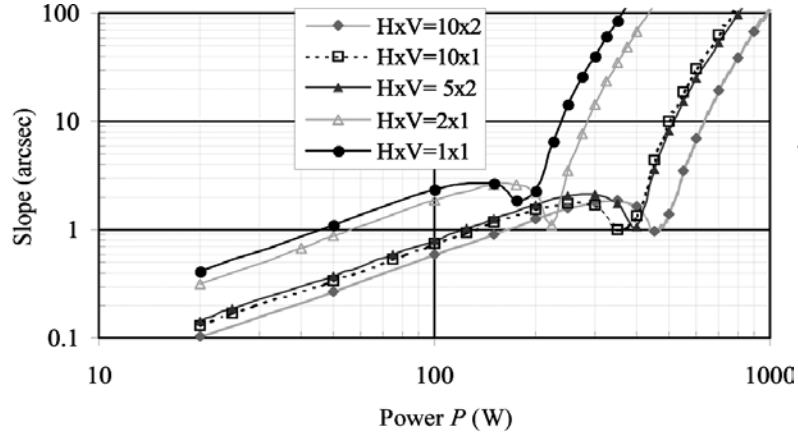
Undulator type	Current (mA)	Slit size (mm^2)	Distance to source(m)	Power (W)	MLPD (W/mm)	X-ray energy (eV)
Planar 25m	100 (25)	0.85x0.85	45	390 (97.5)	310 (77.6)	3600
Planar 5m	100 (25)	1.5x1.5	35	394 (98.8)	178 (44.6)	3600
Helical 25m	100 (25)	0.75x0.75	45	94.5 (23.6)	46.7 (11.7)	8328[a]
Helical 5m	100 (25)	1.3x1.3	35	93.8 (23.5)	26.7 (6.68)	8328[a]
Planar 25m	100 (25)	0.75x0.75	45	136 (34)	69.3 (17.3)	8000[b]
Planar 5m	100 (25)	1.3x1.3	35	135 (34)	39.7 (9.97)	8000[b]

[a]Cornell helical undulators have highest on-axis power at this energy; [b]A case of moderate K number

Studies of LN_2-cooled Si monochromator

- **Internal cooling:** 3 different regions



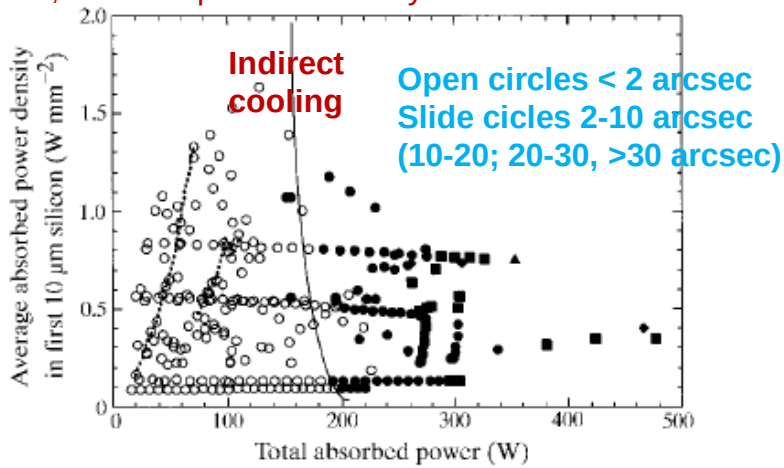


3 regions:
Linear
Transition
Non-linear

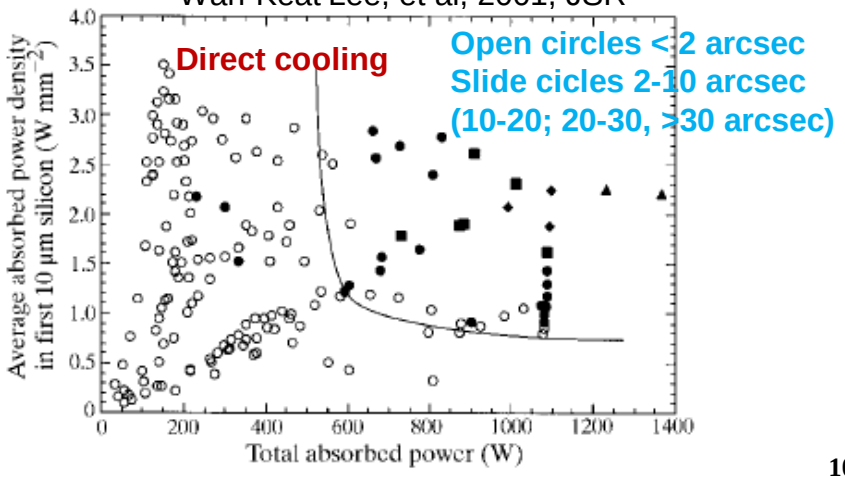
(Lin Zhang, et al., JSR 2003)

- **Affected by both power and power density**

APS 1ID, maximal possible density: 160W/mm²

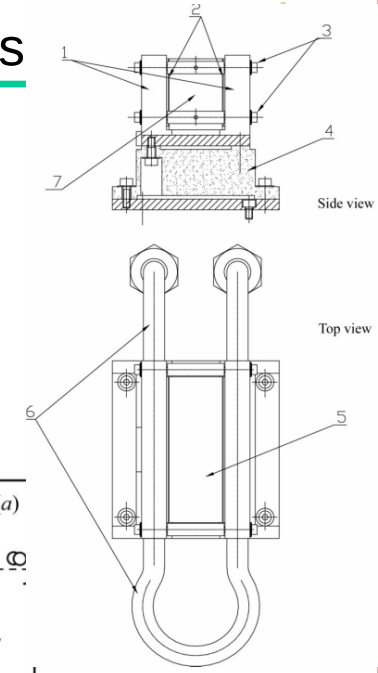


Wah-Keat Lee, et al, 2001, JSR



LN_2 contact cooling, achievements on 3rd generation sources

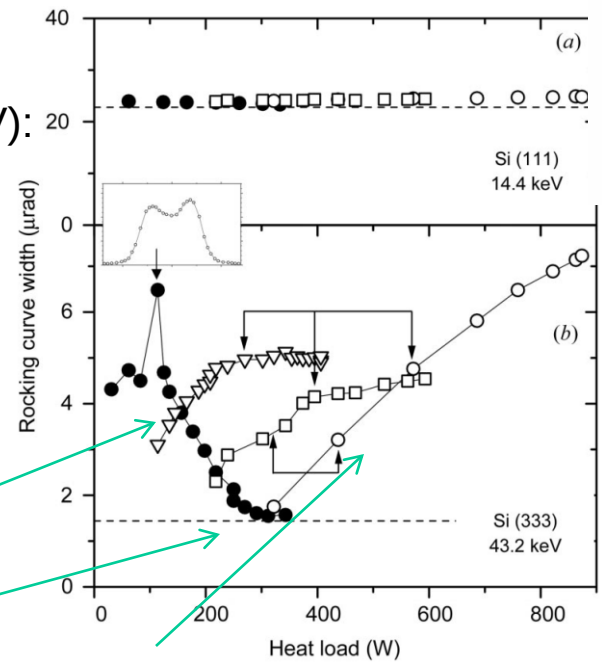
Aleksandr Chumakov, et al, JSR 2004. ("latest", therefore good results)



- Source: ESRF, ID18, three 1.6m long undulators, 32mm periods
- Monochromator distance: 28m
- Maximal power on central cone: ~ 450W (@200mA, 11mm Gap)
  maximal power through front-end: ~1000W
- Si(111), 80L x 30W x 40D (in mm), LN2 contact cooling

Major results (Si(111) ; measurement @ 14.4keV):

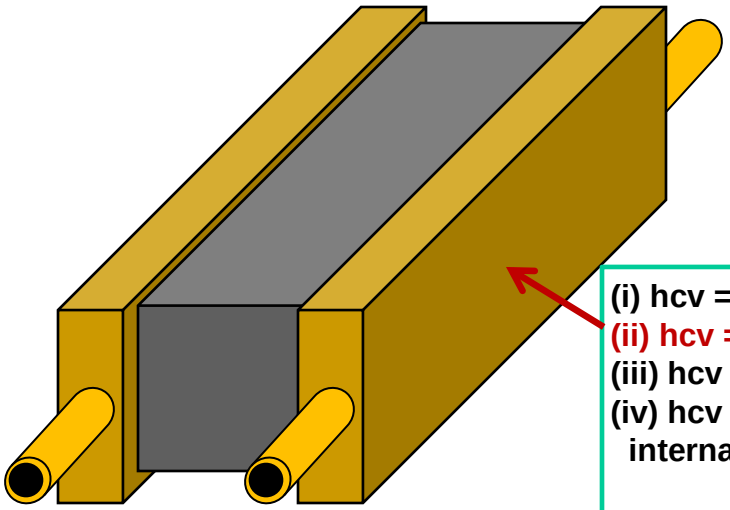
- Mounting deformation & vibration < 0.25 urad
- Ideal performance up to 570W
  @ density up to 210 W/mm^2.
- Acceptable performance up to **900W**.
  (BUT: heating area > central cone)
- Existence of "Si zero expansion region"
  (with rocking curve broadening < 0.8 urad)



Solids: Gap scan of 2 undulators
Very small destortions (~0.8urad) ~340W
opens: Vertical slit scan with horizontal slits at different sizes (1, 1.5, 2mm: circle, square, triangle)

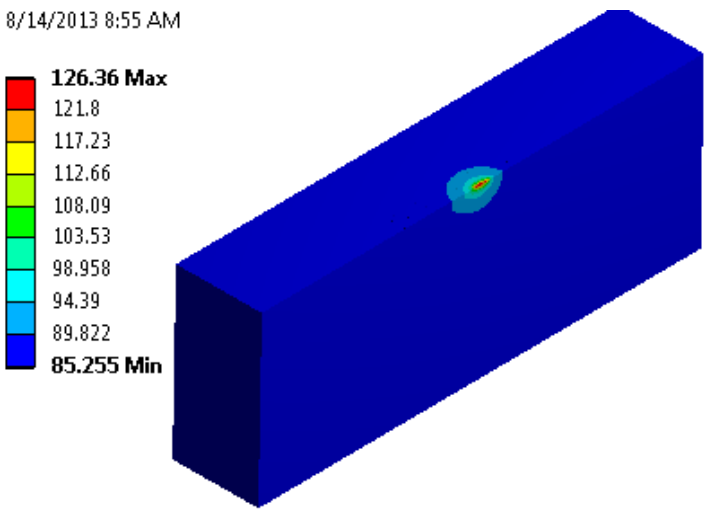
- **Contact cooling gives satisfactory results.**
- **Thermal deformation determined by total power, power density, slits opening etc.**

Assumptions of LN_2-cooled Si crystal for ERL



- Si(111), 30mm × 30mm × 80mm.
- Contact LN_2-cooling from 2 sides.
- moderate effective film coefficient (5000 $Wm^{-2}K^{-1}$).

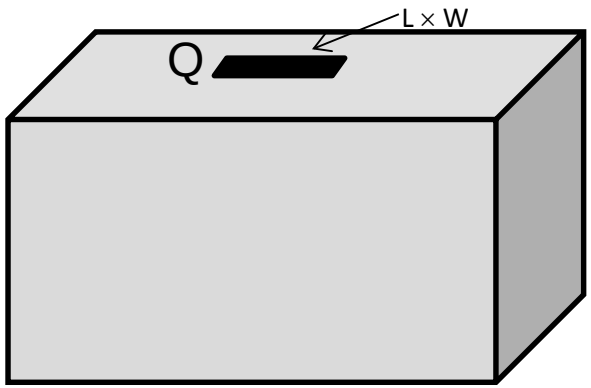
(i) hcv = 3000 W m^{-2} K^{-1} --- fair thermal contact between copper and crystal;
(ii) hcv = 5000 W m^{-2} K^{-1} --- good thermal contact;
(iii) hcv = 8000 W m^{-2} K^{-1} --- excellent thermal contact;
(iv) hcv = 18000 W m^{-2} K^{-1} --- side cooling coefficient equivalent to direct internal cooling system with a cooling coefficient of hcv0 =10000 W m^{-2} K^{-1}.
-- Lin Zhang (ESRF), JSR, 2003



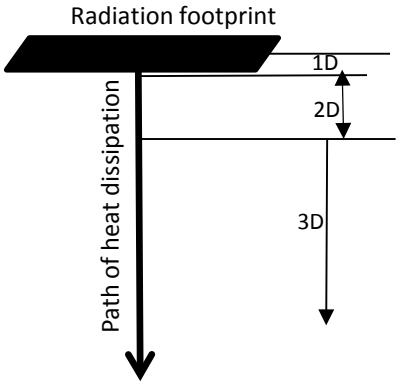
The thermal profile mainly determined by the heat dissipation capability of Si

Simplified analysis model & MLPD

- We estimate thermal conduction in Si crystal with three different approximations at different regions:



(a)



(b)

(L>W)
(crude model)

1D conduction: $dq/dr = 0$, for $r < W/2$

2D conduction with cylindrical symmetry: $d(rq)/dr = 0$, for $W/2 < r < L/2$

3D conduction with spherical symmetry: $d(r^2 q)/dr = 0$, for $L/2 < r < \infty$

where $q = -K(T)\, dT/dr$

- Analytical analysis of cryogenic Si Laue monochromator by B.X.Yang (1993), using approximation of Si thermal conductivity (SPIE, 1993):

$$K(T) = A/(T - T_k)$$

with A=44.63 W/mm, and T_k=47.4K.

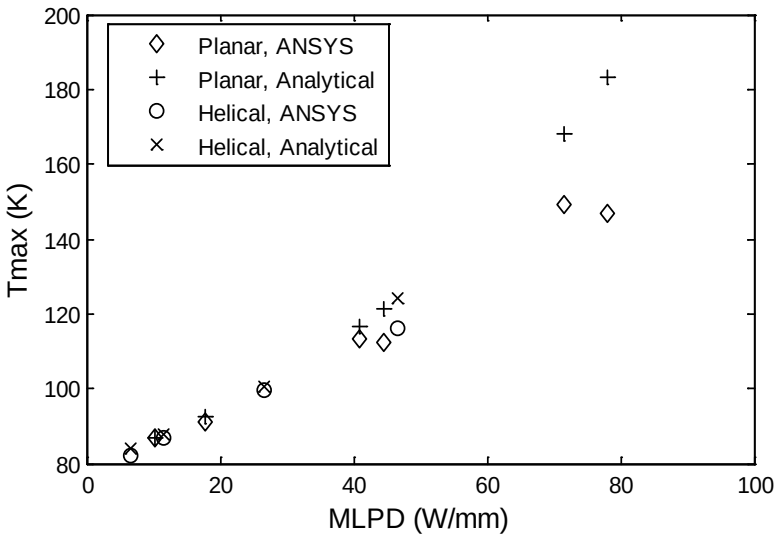
- With assumption of T=T0 at far away from footprint: → $T = T_k + (T_0 - T_k)\exp(0.0183 P_M)$ where:

$$P_M = [1 + ln(L/W)/2.571]Q/L$$

We call it modified linear power density **(MLPD)**

Comparison of Tmax with simulated Tmax

- Comparison of Tmax estimated analytically with Tmax simulated using ANSYS, for Cornell ERL undulators. (Tmax > room temperature are ignored)



Use MLPD as metric for Si thermal deformation

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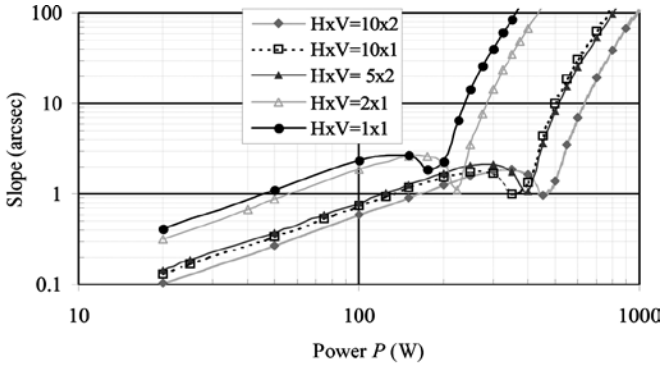
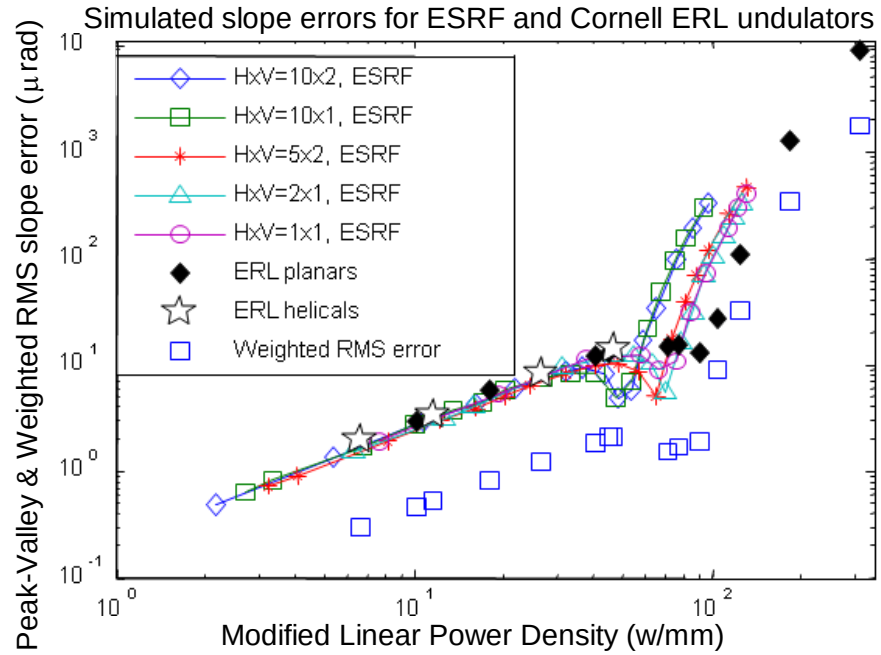
- Parameterizing thermal deformation with MLPD



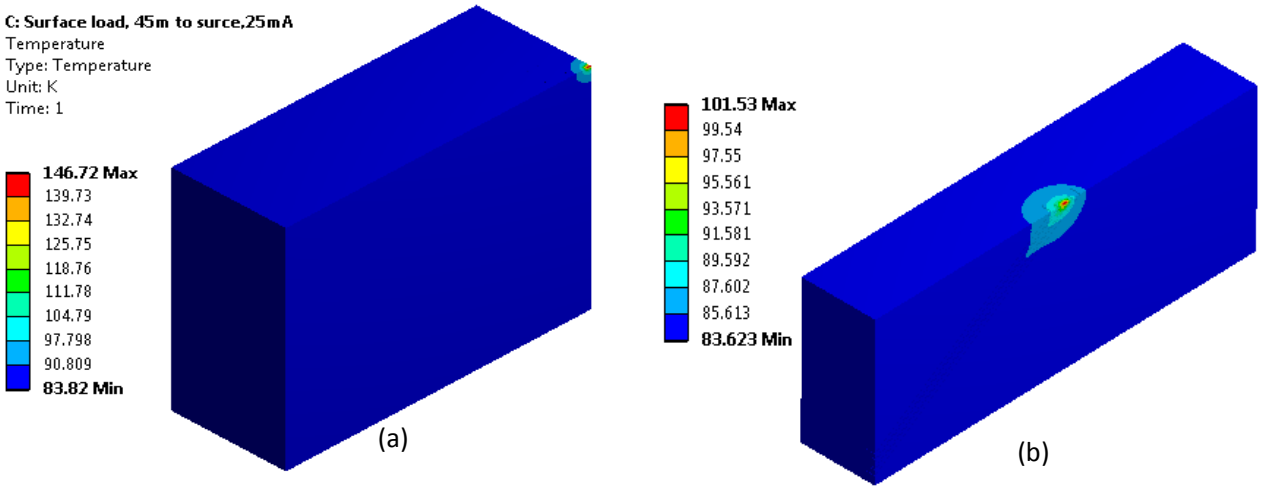
& Our ANSYS results for ERL



- We suggest "X-ray intensity weighted RMS slope errors, $\alpha_{RMS} = \sqrt{\left\{\int I(x)[E(x) - mean(E(x))]^2 dx\right\} \Big/ \int I(x)dx}$ (blue squares in figure), better comparable to experiments

- Linear region: MLPD ≤ 50 W/mm
- Transition region: MLPD = 50 – 100 W/mm
- start of nonlinear region: MLPD ~ 100W/mm.

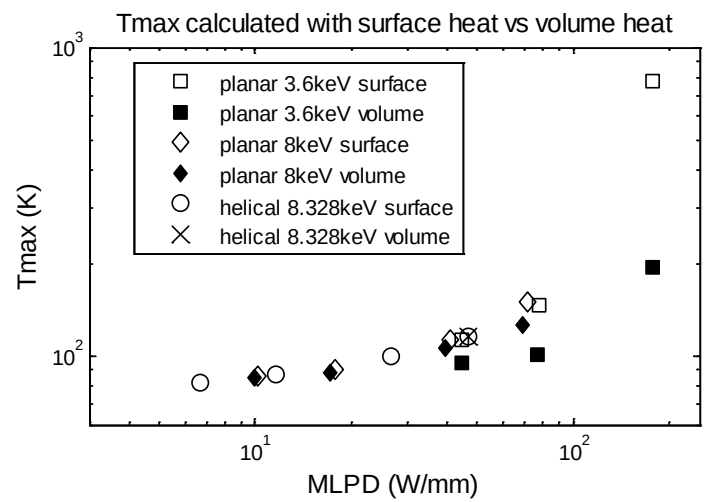
Volume heat effect



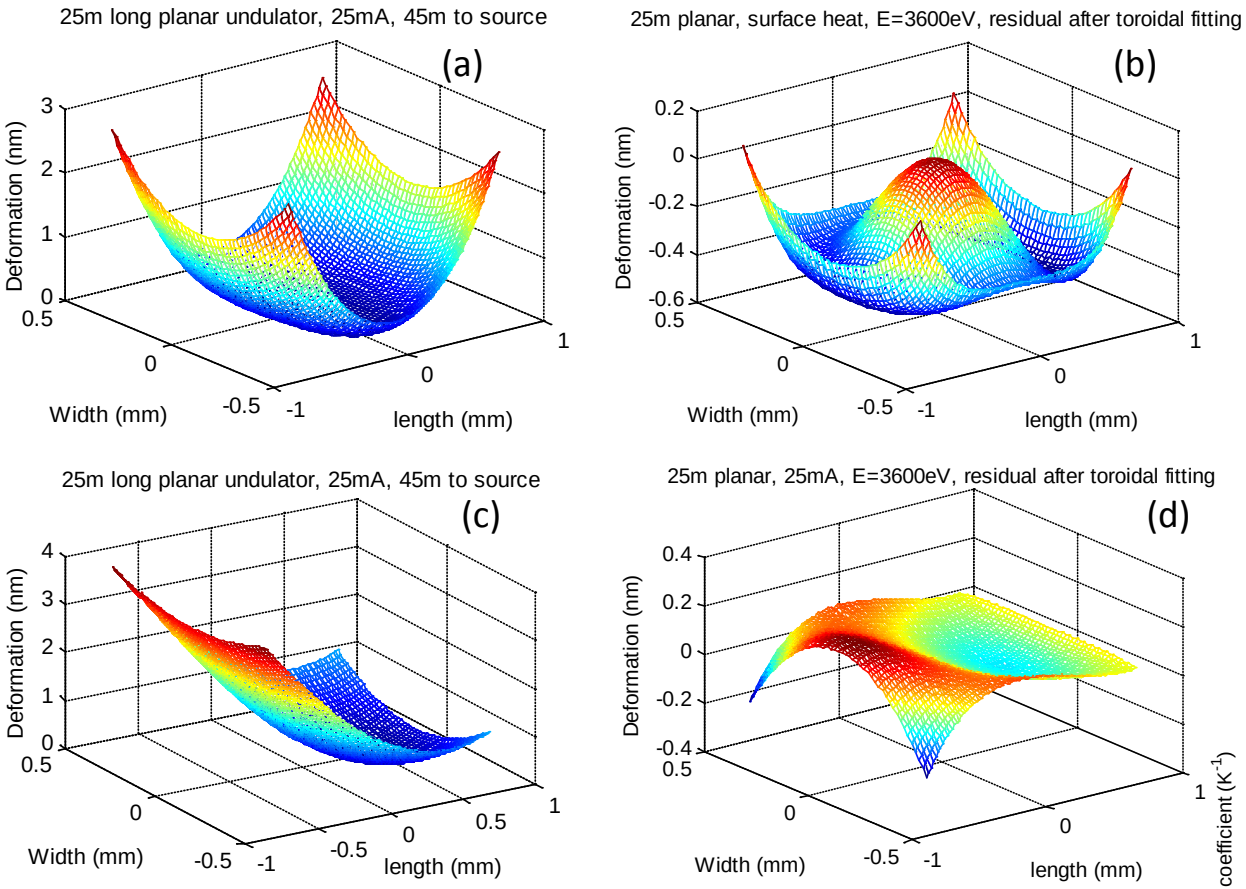
25m undulator, 3.6keV (K=2.22);
High coherent mode (25 mA);
Mono at 45m from source;
slit size 0.85mm by 0.85 mm;
power: ~98 W

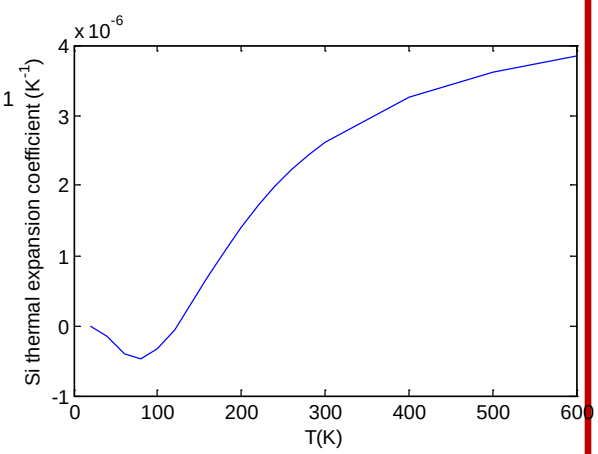
- Significantly decreased the calculated Tmax, for planar undulator at high K;
  less significant for planar at lower K
  (such as 8keV, K=1.06);
  negligible for undulator at helical polarization.

- Asymmetric temperature profile and asymmetric deformation



- Volume heat → asymmetric deformation even after "rock curve position" correction and "toroidal focusing" subtraction





- Si deformation will mostly cause thermal "dip" (thermal expansion <0 when T<125K)

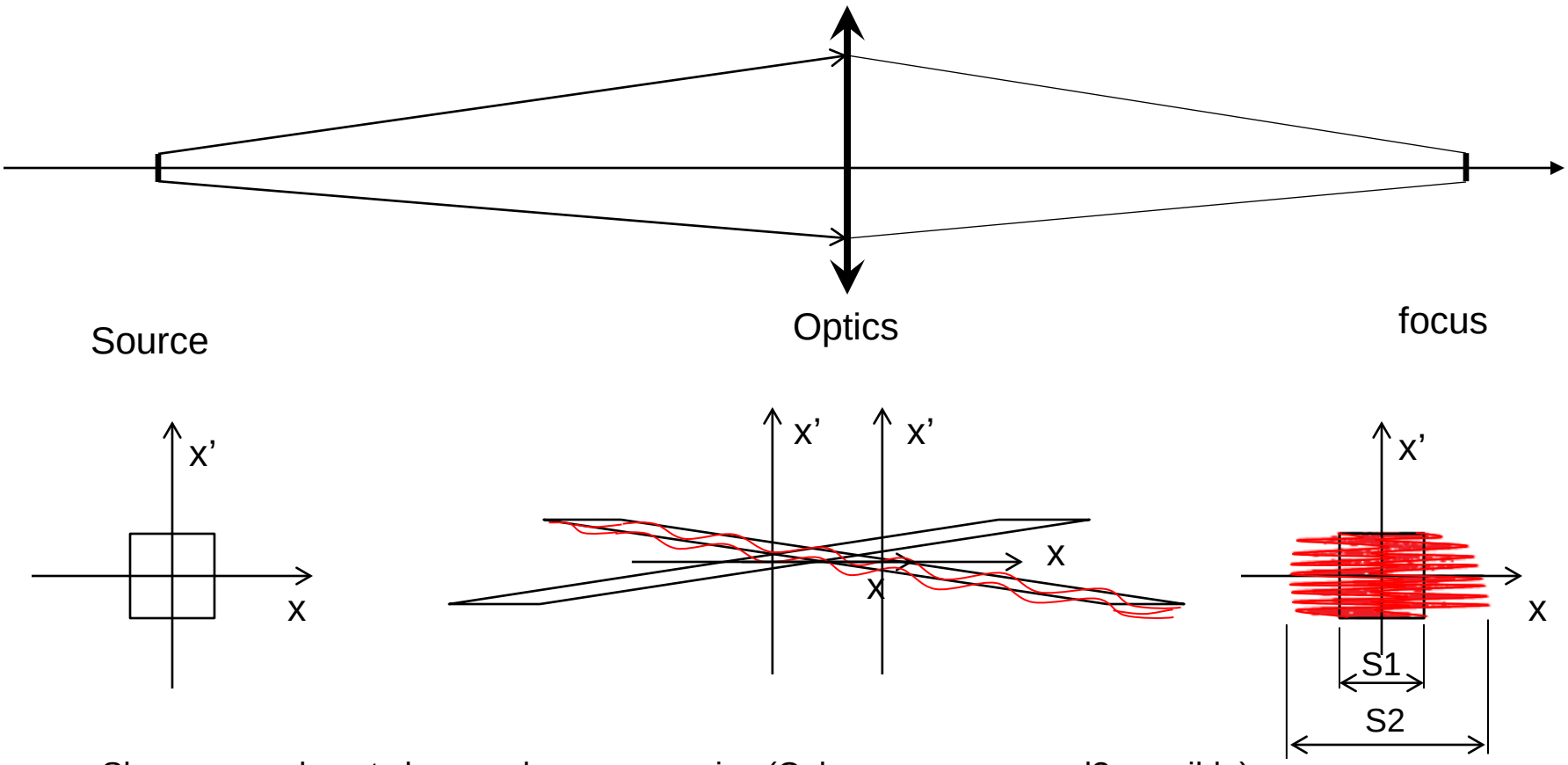
Deformation for Cornell ERL beamlines (using volume heat load)

- Small deformation for both 5m and 25m "helical undulators", under any "gap"
- Small deformation for both 5m and 25m "planar undulators" working at "normal" K (deflection parameter)
- Small deformation for any undulators working at coherent mode (25mA machine current)
- Improvement needed for "planar undulators" work at high flux mode at "closed gap"

Distance to source (m)	Beam current (mA)	Slit size (HxV) (mm x mm)	Foot print (mm x mm)	Total power[3] (Watt)	Power density[4] (W/mm^2)	Modif. Lin. Pow. Den. (w/mm)	Tmax (K) Ansys/Estimated	P-V slope error (arcsec)	I_weighted RMS errors(urad) (x–directions)
25m planar undulator, 3.6keV									
45	25	0.85 x 0.85	0.85x1.547	97.43	134.8	77.62	101.5	1.411	1.348
	100	0.85 x 0.85	0.85x1.547	389.5	539.1	310.3	311.1	66.69	80.04
5m planar undulator, 3.6keV									
35	25	1.5 x 1.5	1.5x2.73	98.8	43.91	44.60	95.2/	1.019	0.898
	100	1.5 x 1.5	1.5x2.73	393.9	175.1	177.8	193.7/	10.4	12.5
25m planar undulator, 8keV									
45	25	0.75 x 0.75	0.75x3.034	34.0	60.4	17.30	88.56/	0.696	0.607
	100	0.75 x 0.75	0.75x3.034	136.1	242.0	69.3	126.36/	2.399	1.94
5m planar undulator, 8keV									
35	25	1.30 x 1.30	1.30 x 5.26	33.96	20.1	9.97	85.48/	0.4185	0.3527
	100	1.30 x 1.30	1.30 x 5.26	135.15	79.97	39.66	106.55/	1.771	1.467
Helical undulators (mostly surface load)									
45 (25m)	25	0.75x0.75	0.75x3.159	23.62	41.975	11.66	86.93/87.75	0.700	0.525
	100	0.75x0.75	0.75x3.159	94.47	167.9	46.64	116.0/123.9	2.90	2.047
35 (5m)	25	1.30x1.30	1.3x5.476	23.46	13.78	6.68	82.26/84.24	2.24	0.295
	100	1.30x1.30	1.3x5.476	93.83	55.51	26.72	99.79/100.6	1.71	1.246

How Si thermal deformation may affect beam quality

A simple analogy using geometric optics



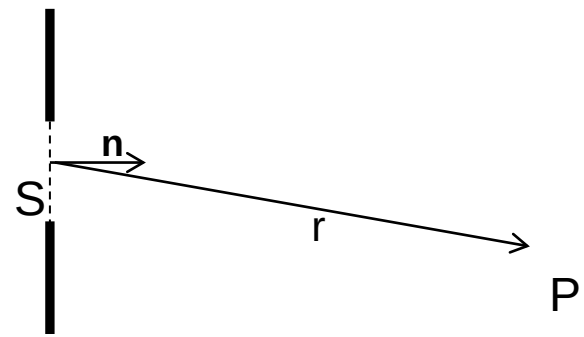
- Slope errors do not change phase space size (Coherence preserved? possible)
- It changes optical size (S1 → S2).
- ERL small emittance is advantageous for high flux nano-focusing, will the small monochromator thermal deformation ruin this advantage?

Wave propagation through deformed crystal

Kirchhoff's diffraction theory:

$$U(P) = \frac{1}{4\pi}\int_S \left[U\frac{\partial G}{\partial n} - G\frac{\partial U}{\partial n}\right] ds$$

U: a component of field amplitude, G can be $\frac{e^{ikr}}{r}$ etc.



Which can be equivalent to Huygens-Fresnel Principle:

$$U(P) = \frac{-i}{\lambda}\int_S U\frac{e^{ikr}}{r}\vec{n}\hat{r}\, ds$$

If there is an optical element at S location:

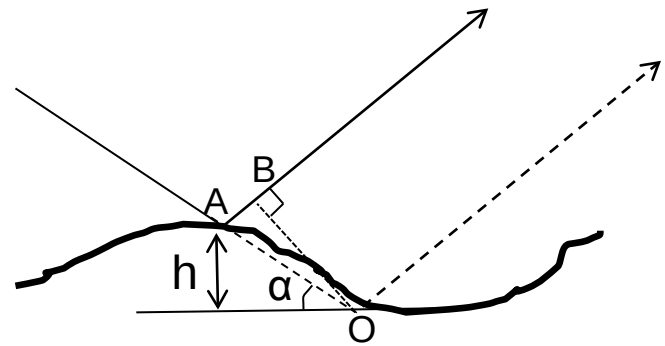
$$U(P) = \frac{-i}{\lambda}\int_S UT(x,y)\frac{e^{ikr}}{r}\vec{n}\hat{r}\, ds$$

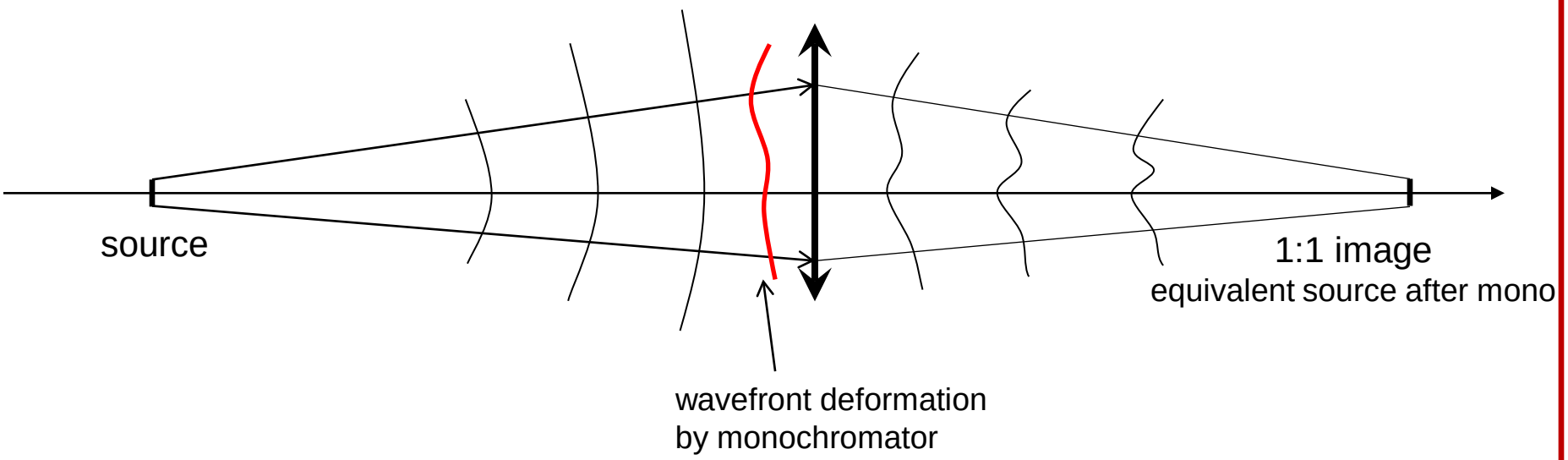
T(x,y) describes the change of field amplitude and optical path by optical element with area S

Synchrotron Radiation Workshop was used for the simulation.

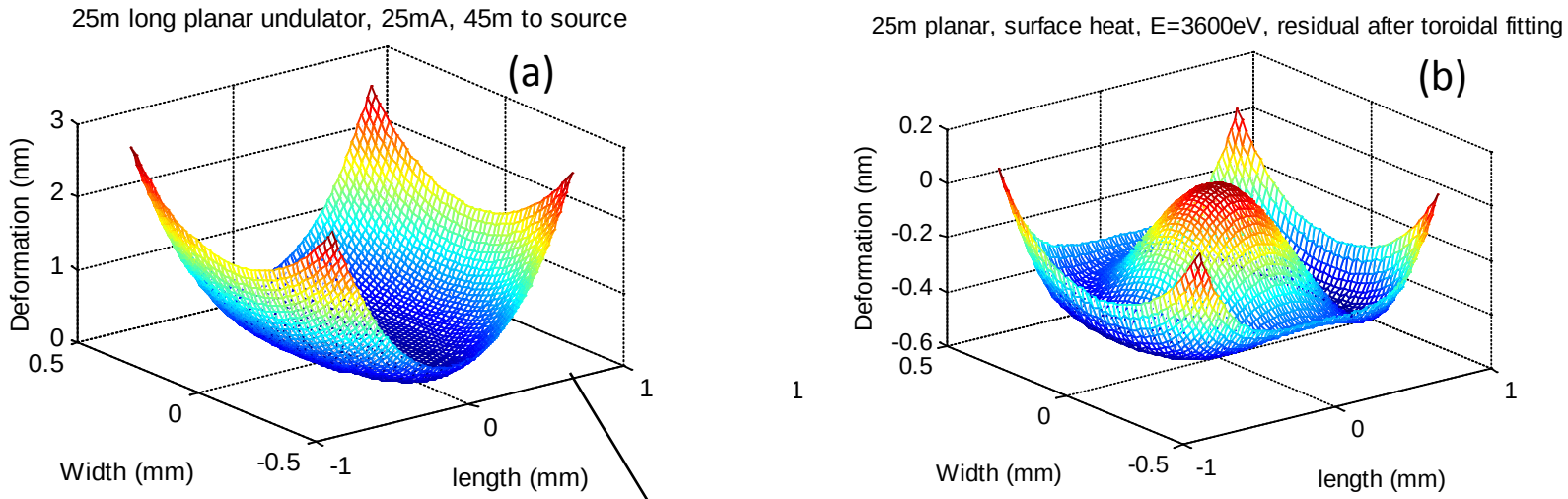
Evaluate wavefront deformation effect by 1:1 focusing

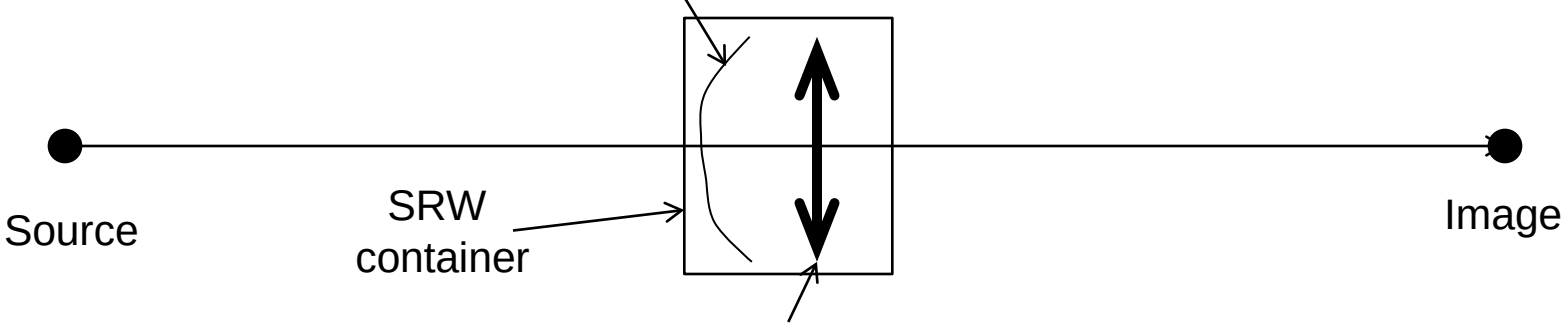
- Slope errors much less than rocking curve width
  → No change of dynamic diffraction
- Slope errors affects X-ray phase shift locally.
  The path length change as show in figure:
  $\overline{OA} - \overline{AB} = 2h \times sin(\alpha)$
- Thin optics assumption
  (transverse position shift by mono is negligible)





For real1:1 focusing, “thermal curvature” has to be subtracted

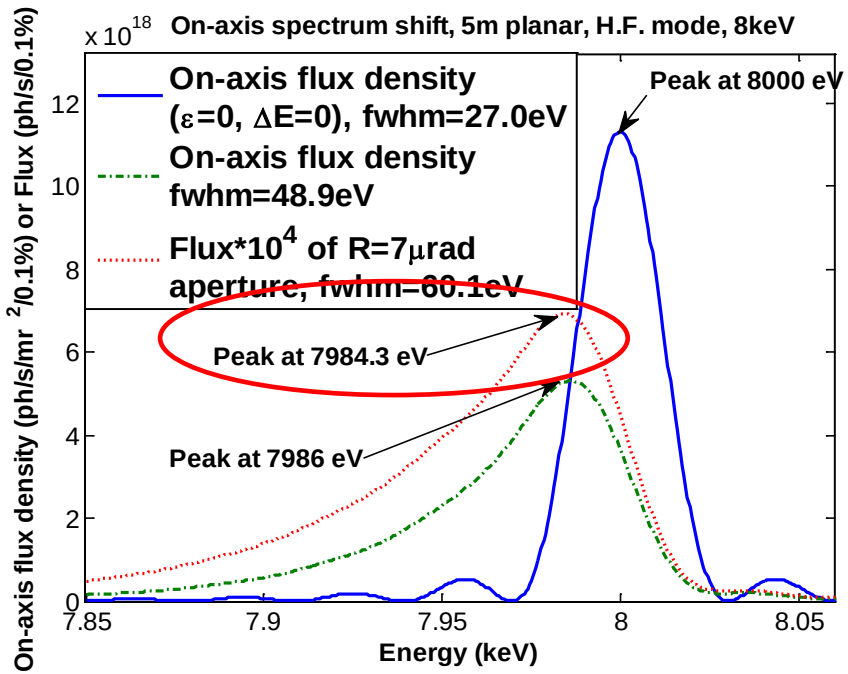




$$\frac{1}{f_{x,y}} = \frac{1}{f_{1:1}} - \frac{1}{f_{x,y_thermal_curvature_toroidal_fitting}}$$

SRW simulation at the peak of on-axis spectrum

- Simulations were done at the energy of on-axis spectrum peak



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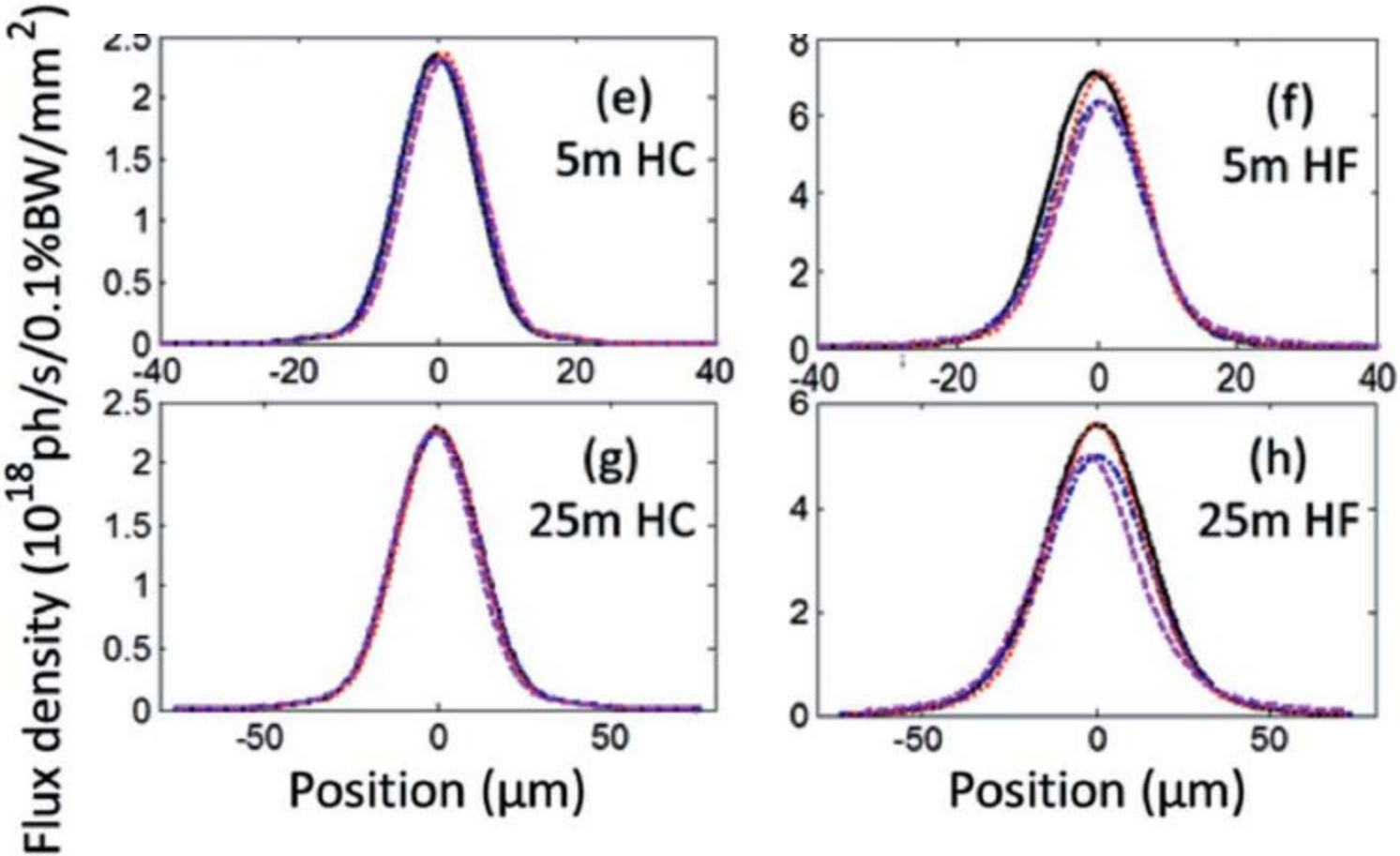
Undulator type	First-harmonic energy (keV)	Current (mA)	Residual error (Å)†	Focus without deformation		Focus with deformation	
				$FWHM_x$ (μm)	$FWHM_y$ (μm)	$FWHM_x$ (μm)	$FWHM_y$ (μm)
5 m planar	8.0	25	1.81/0.20	12.9	12.6	12.9	12.7
	8.0	100	6.77/0.78	15.4	14.4	15.9	15.2
25 m planar	8.0	25	1.94/0.23	28.4	27.5	28.7	27.4
	8.0	100	3.74/0.59	35.0	32.4	35.1	34.0
5 m helical	8.32	25	1.11/0.18	13.1	12.9	13.2	12.9
	8.32	100	4.74/0.77	15.4	14.2	15.6	14.7
25 m helical	8.32	25	1.31/0.19	28.8	27.9	29.2	27.8
	8.32	100	4.71/0.74	34.7	32.1	34.8	33.2

† Peak-to-valley/RMS values of the thermal displacement after subtraction of toroidal curvatures.

Results for helical undulators @ 8.32keV (maximum radiation power)



HC: high coherence mode; HF: high flux mode
solid, dotted: H & V profile without deformation
Dash-dotted, dashed: H & V with thermal deformation

Results for planar undulators @ 8.0keV (not maximum power but more realistic)

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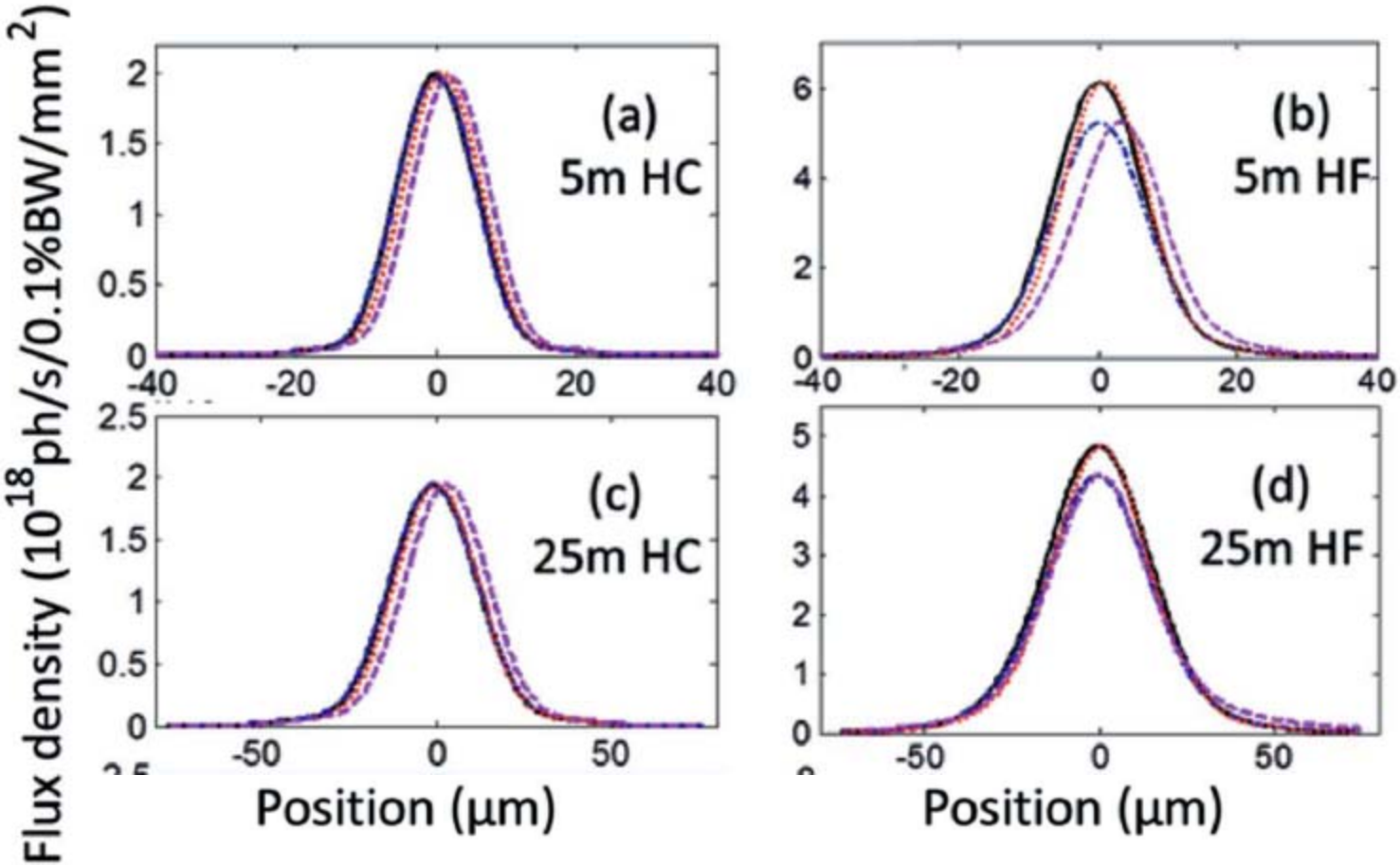

HC: high coherence mode; HF: high flux mode
solid, dotted: H & V profile without deformation
Dash-dotted, dashed: H & V with thermal deformation

Cryogenic mono: scattering – seems well known and well taken care of

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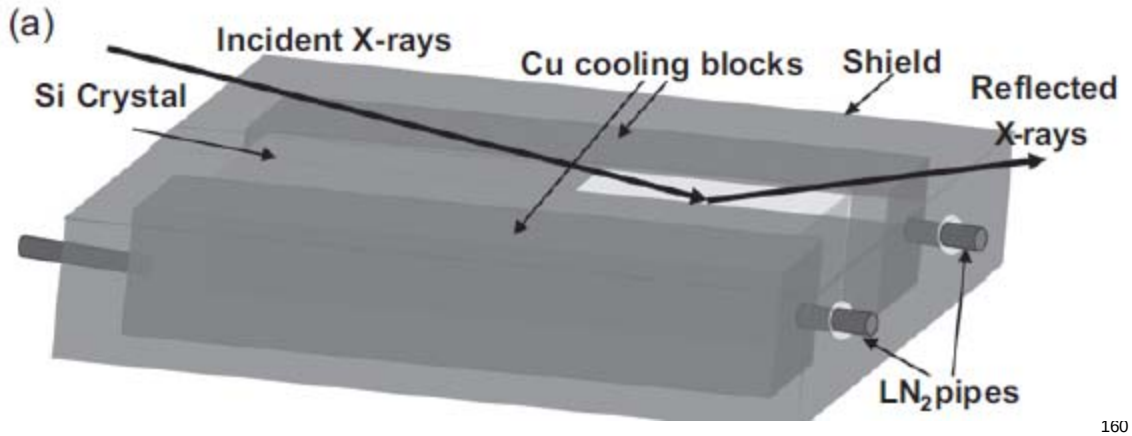
- Well known the importance of scattering shielding.
- Widely used in almost every monochromator.
- Feedback takes care the rest after shielding.

- Only few pays attention to scattering:
  Eleonora Secco and Manuel Sanchez del Rio: "*Monte Carlo simulations of scattered power from irradiated optical elements*" **SPIE** 2011
  - Python interface for PENetration and Energy Loss of Positrons and Electrons (PENELOPE)
  - Simulated scattering from Glidcop mirror, Si crystal, Laue crystal

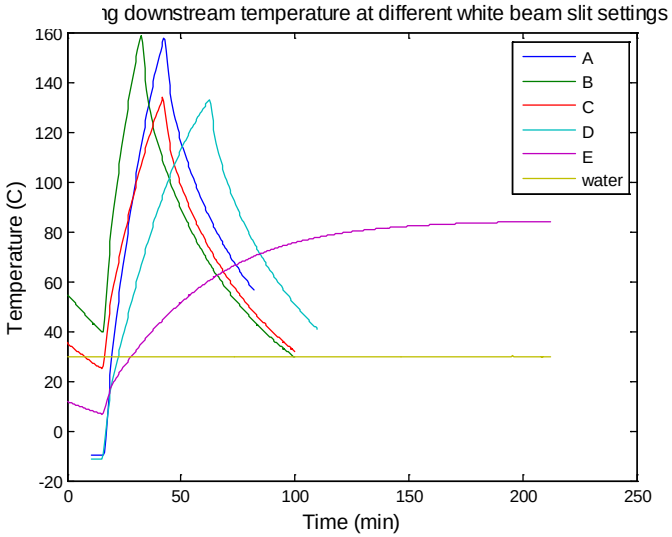
- Quantitative study of scattering might be useful for high energy and high current beamline in specific cases

Cryogenic mono for 17ID upgrade (~2009)

Tested at maximum heat condition:
- Closed gap (11.0mm, K~2.5)
- Si(111) mono around 10 keV

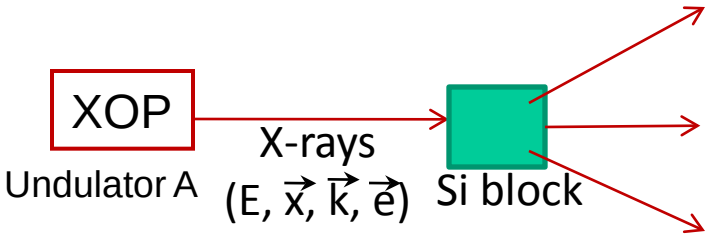


Crystal: 30x30x150



Initial testing: shield overheated !

Monte Carlo simulation of scattering

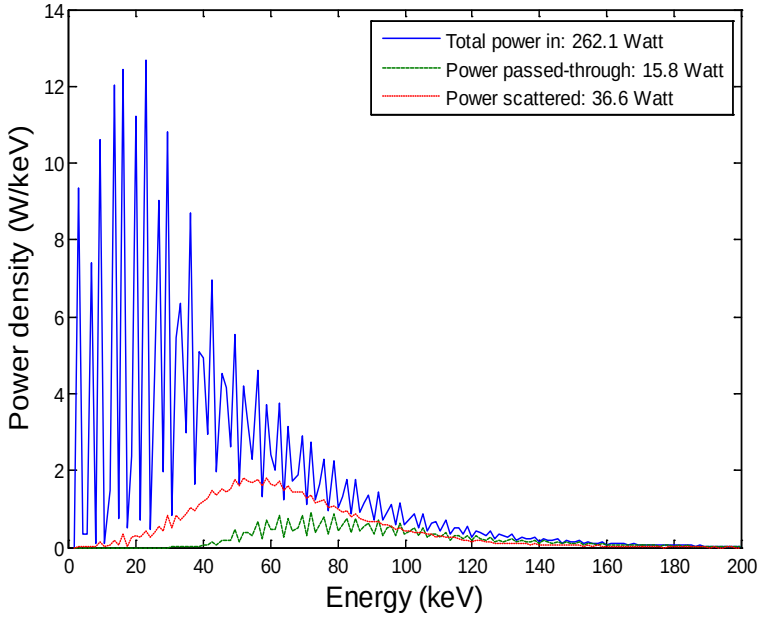


Photoelectric (K shell X-rays)
(E, $\vec{x}$, $\vec{k}$, $\vec{e}$)

Coherent Scattering
(E, $\vec{x}$, $\vec{k}$, $\vec{e}$)

Incoherent Scattering (& depolarization)
(E, $\vec{x}$, $\vec{k}$, $\vec{e}$)

Energy Spectrums of Incident, Passed-Through and Scattered X-rays



Very high percentage of scattered power **>50keV!**

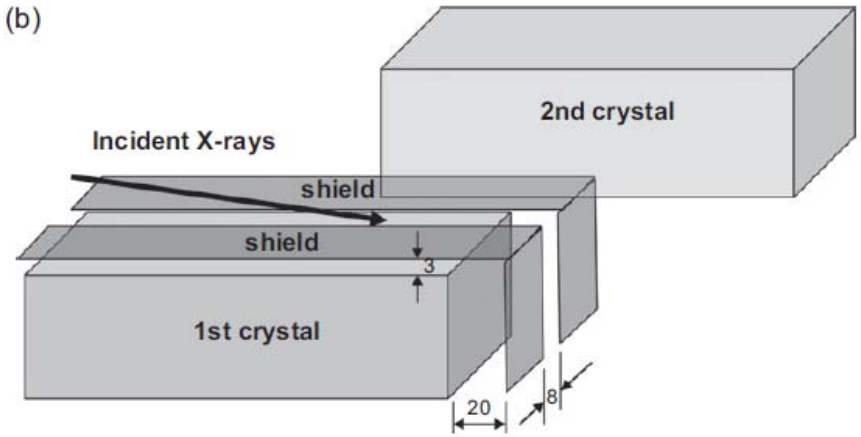
Half intercepted power is transmitted beam:
Should never "shield" transmitted beam !!

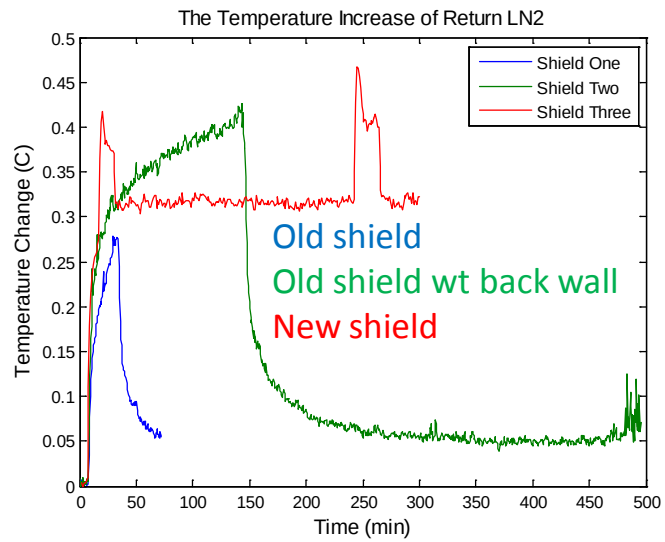
Beam size: 1x1.7, incident power:	**262W**
Total "out-of-crystal" power:	**52.4W**
Shield intercepted power:	**32.0W**
Transmitted power:	**15.8W**
Shield T increase: ΔT≈ 376 deg	

Remove downstream shield: **ΔT≈ 133 deg**
measured ΔT≈ 130 – 140 deg

Shield with small thermal resistance

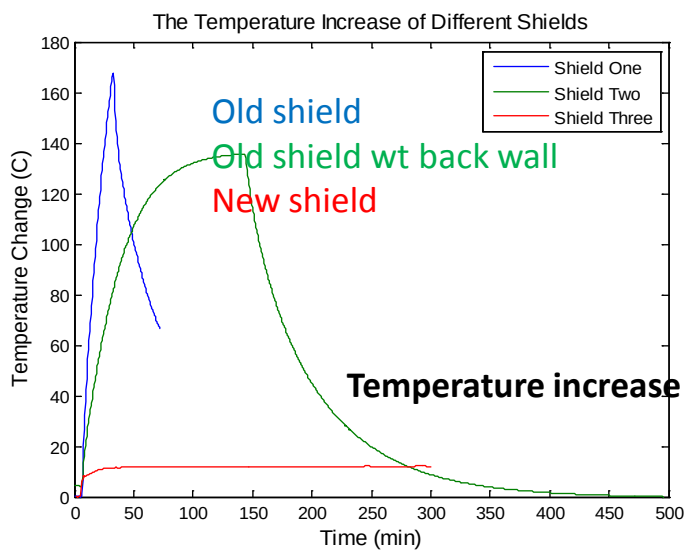
Connect to LN2 block through spacer



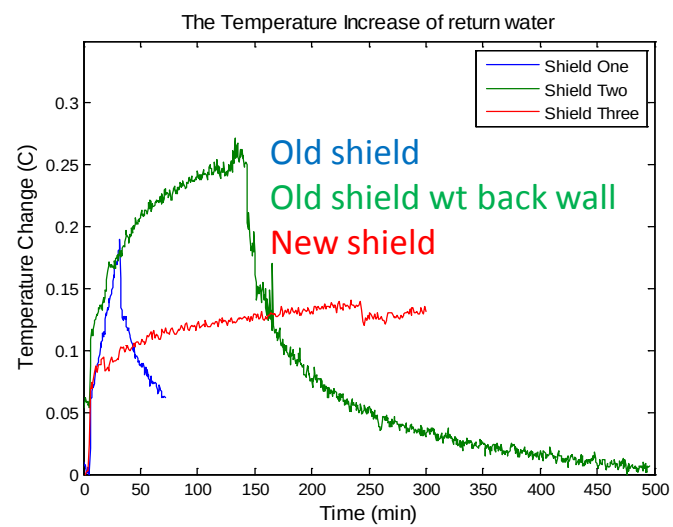


Temperature change on return LN2

Temperature change on return water



Temperature increase on shield



Conclusion

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- **For Cornell ERL beamlines, cryogenic monochromator is good for:**
  Both 5m and 25m "helical undulators", under any "gap";
  Any undulators work at coherent mode (25mA machine current) ;
  Both 5m and 25m "planar undulators" working at "normal" K.

- **Improvement needed for "planar undulators" work at high flux mode at "closed gap".**
  (But will be fine if working at 3rd harmonic E=10.8keV, at 55m, where MLPD=114 W/mm)

- **Wavefront distortion negligible or very minor from focusing perspective:**
  negligible effect on high coherence mode (25mA, helical @maximum power; planar @ 8keV);
  minor effect on high flux mode (100mA, helical @ maximum power; planar @ 8keV)

- **MLPD should be used to gauge thermal deformation. (not total power, not power density)**

- **For high energy beamline, thermal scattering could affect LN2 mono performance.**

ACKNOWLEDGMENT

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Oleg Chubar (NSLSII) help on using SRW

Don Bilderback (CHESS)

Ken Finkelstein (CHESS)

Ivan Bazarov (Cornell University)

Daren Dale (CHESS)

Mati Meron, Jim Viccaro, (ChemMat CARS)
Lisa Keefe, Lewis Muir, Kevin Battaile, Anne Mulichak (IMCA-CAT)