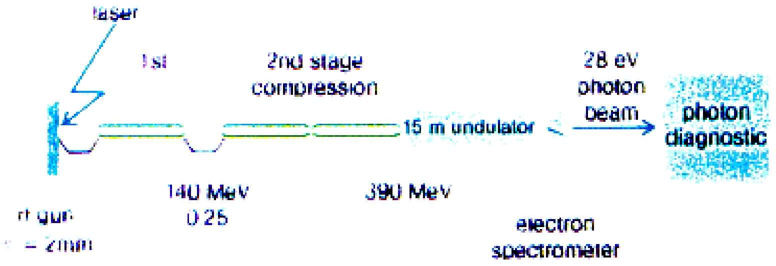
17TH ADVANCED BEAM DYNAMICS WORKSHOP ON
FUTURE LIGHT SOURCES

The X-ray Scientific Case

G. Materlik, DESY

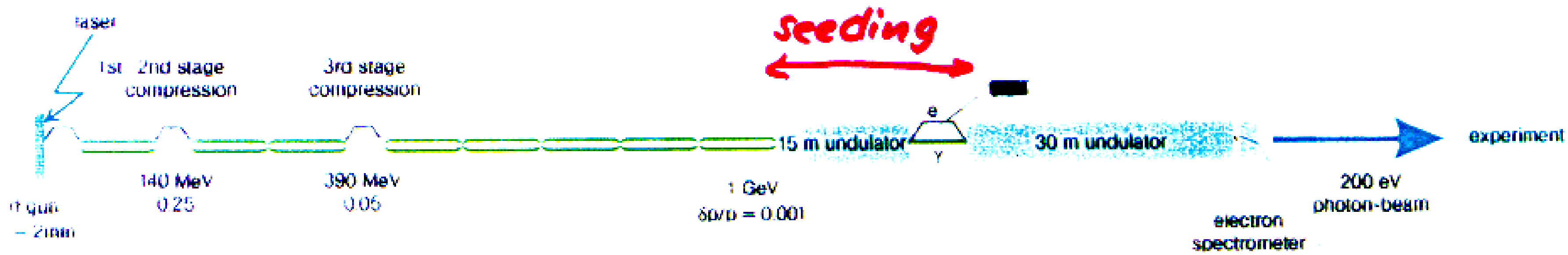
APRIL 6-9, 1999
ARGONNE NATIONAL LABORATORY, ARGONNE, IL U.S.A.

SASE - FEL development at DESY, Hamburg



proof of principle experiment

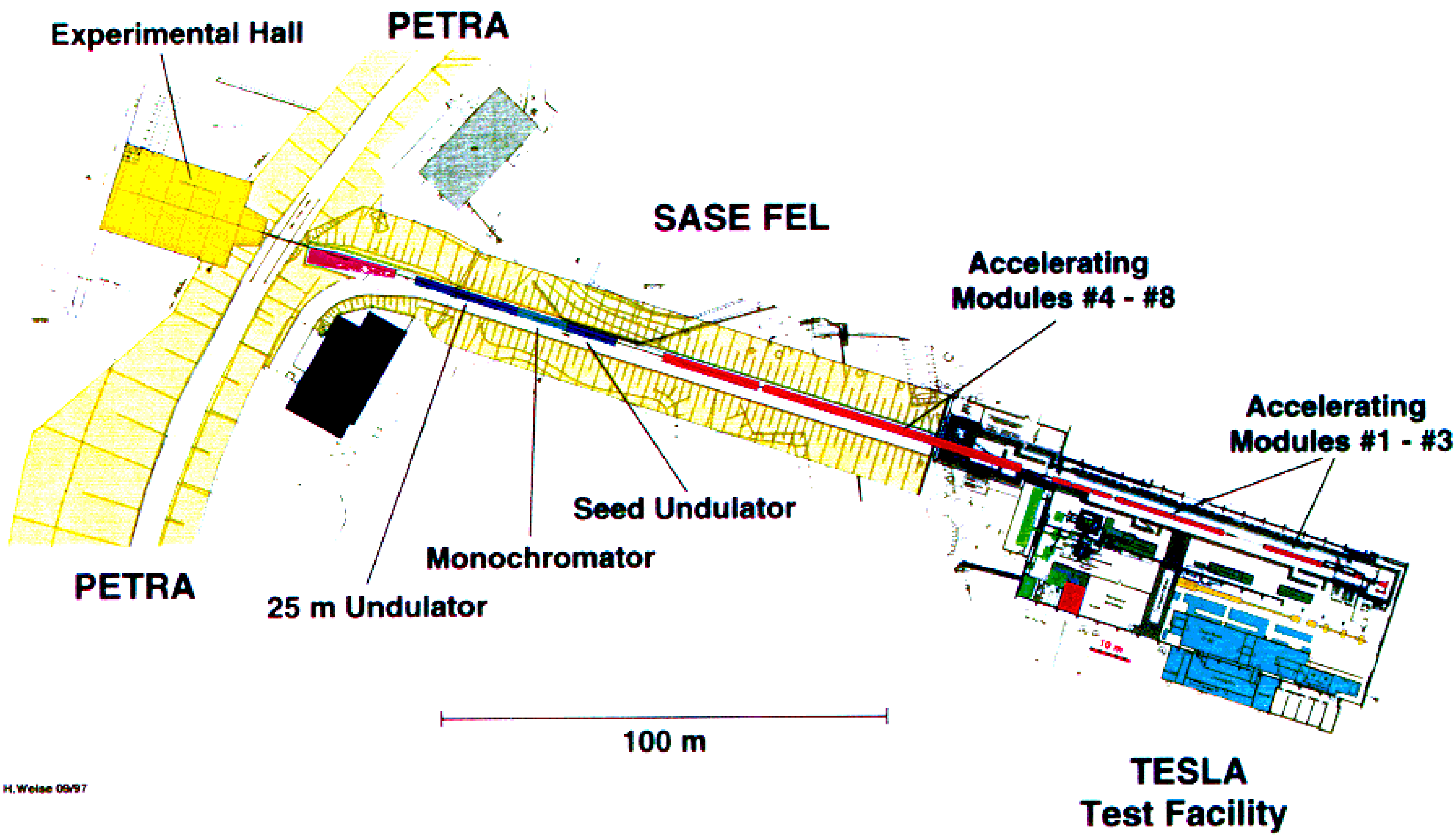
$\lambda \sim 70$ nm   summer 1999



VUV - FEL facility at DESY   end of 2002 →

$\lambda \gtrsim 6\ (2)$ nm

TESLA – VUV FEL Phase I



Ausstellung Exhibition
1. Juni - 31. Oktober

2000
in Hamburg

Licht der Zukunft
Light **for the New Millennium**

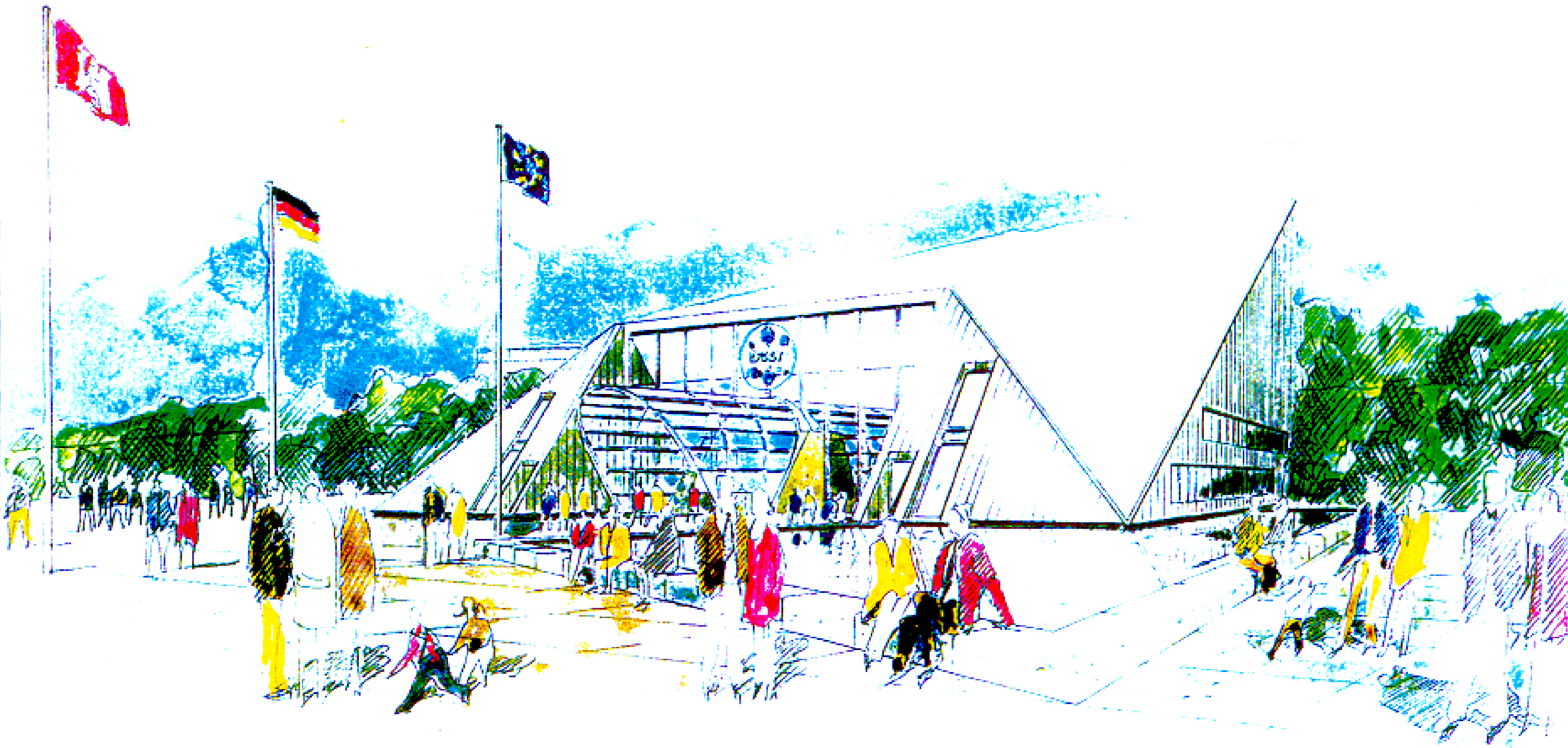
Ein 300 Meter langes supraleitendes
Röntgenlaser-Mikroskop beim
Forschungszentrum DESY
Weltweites Projekt der EXPO 2000

A 300 Meter Long Superconducting
X-Ray Microscope at the
Research Center DESY
Worldwide Project EXPO 2000

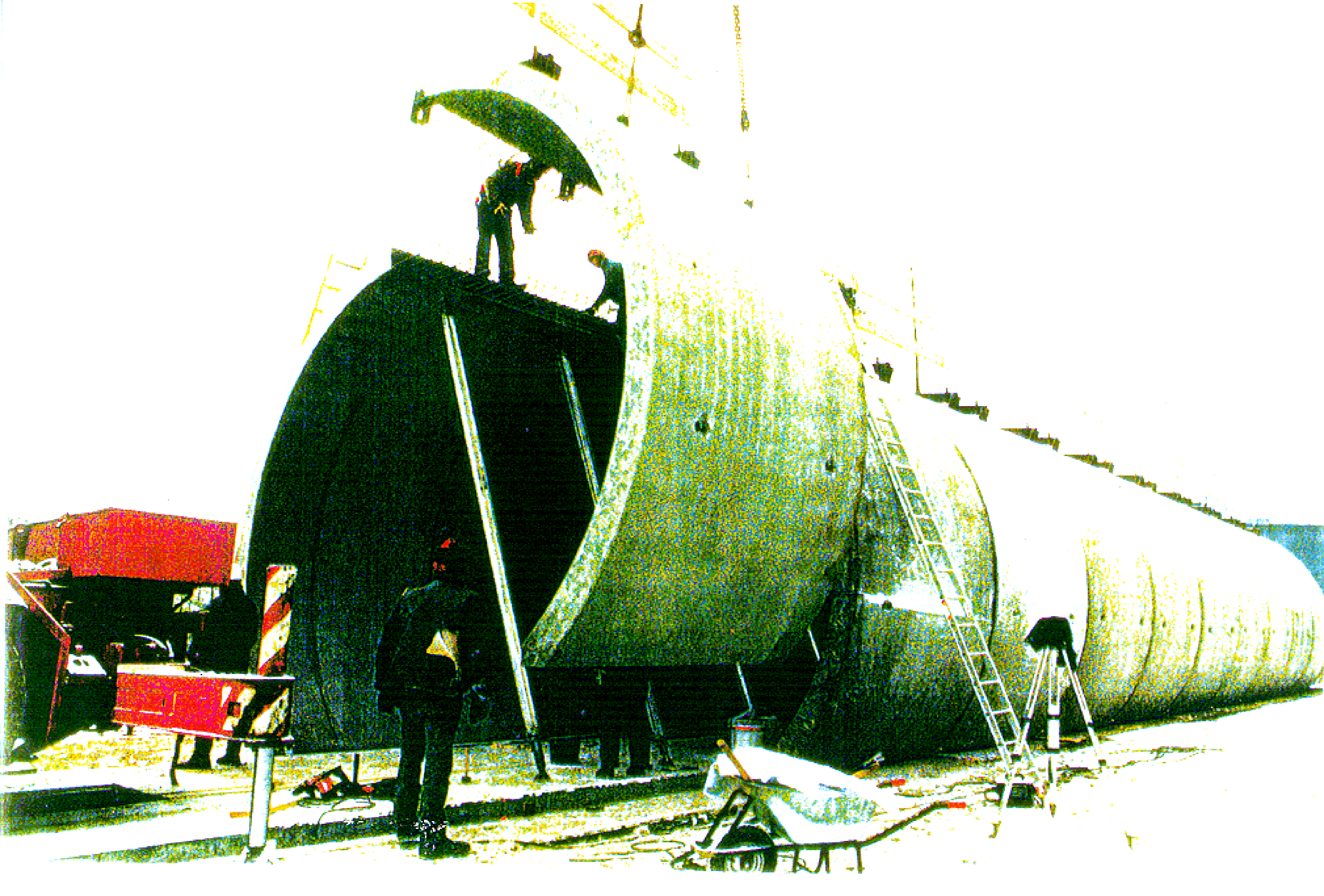
Täglich 10 bis 19 Uhr
Donnerstag bis Mitternacht
Eintritt frei

Daily 10 a.m. to 7 p.m.
Thursday until Midnight
Admission free

www.desy.de/expo2000/



DESY VUV-FEL: Experimental hall EXPO 2000



Conceptual Design of a 500 GeV e^+e^- Linear Collider with Integrated X-ray Laser Facility

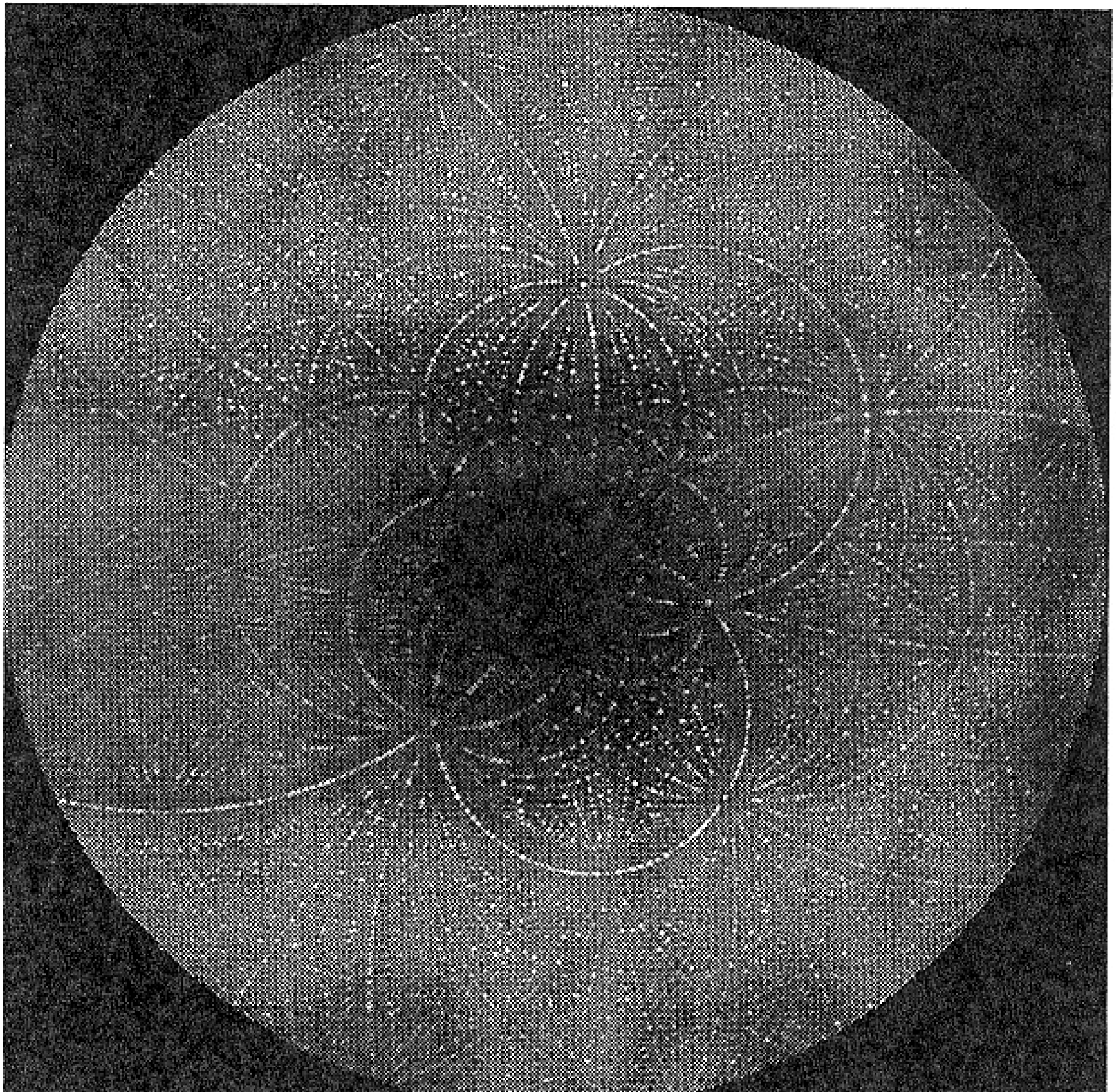
Volume II

Editors:
R. Brinkmann
G. Materlik
J. Rossbach
A. Wagner

DESY 1997-048
ECFA 1997-182

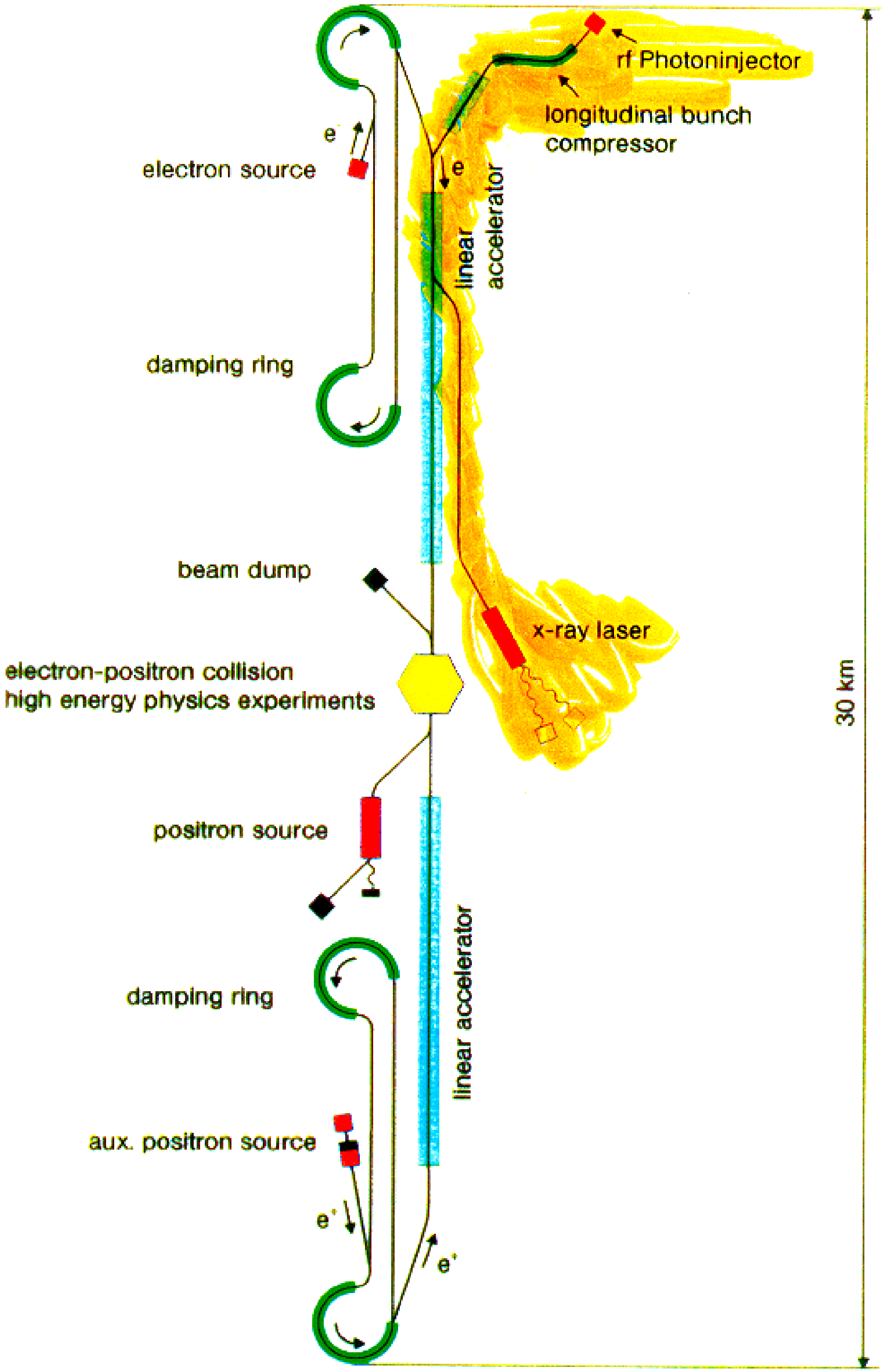
WWW.DESY.DE
FEL

Pages 879 - 940 Scientific case

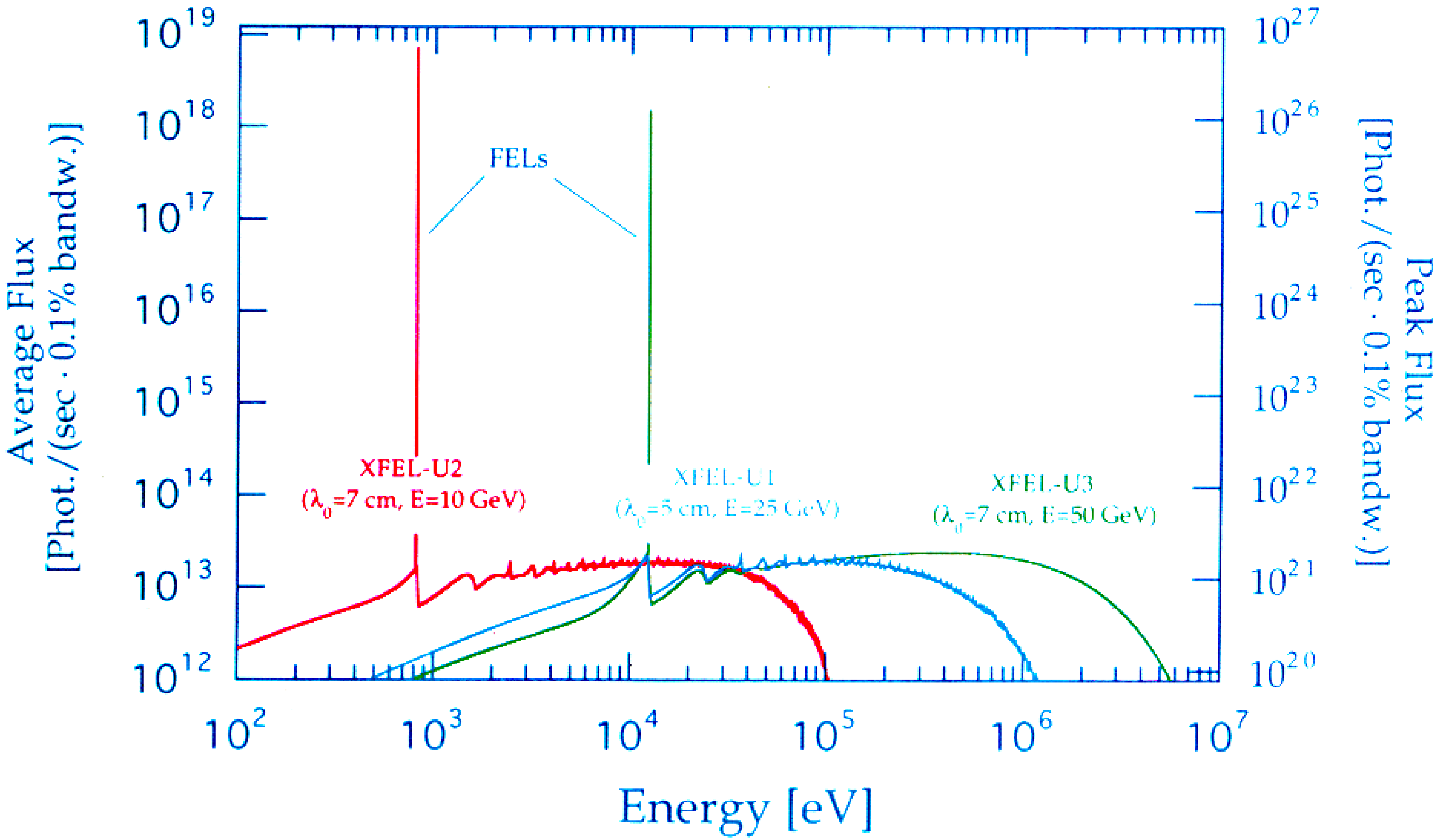


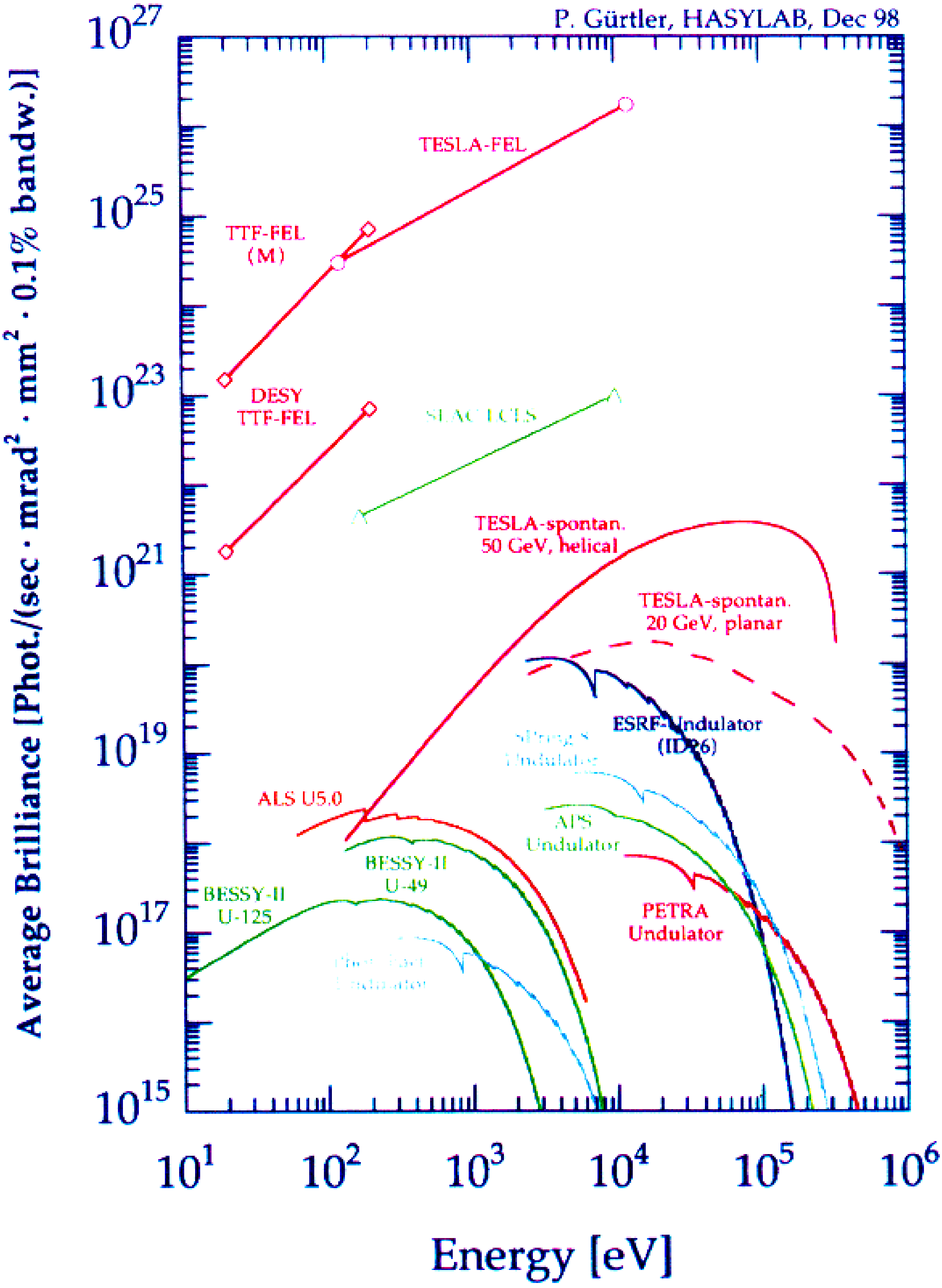
TOP: *Laue diffraction pattern from cubic 2Mn-catalase (Bourenkov, Barynin, Bartunik). The XFEL will permit to record such exposure within 100 fs for time resolved investigations of rapid conformational transitions.*

TESLA Linear Collider with integrated X-FELs



Flux of the XFEL-Undulators

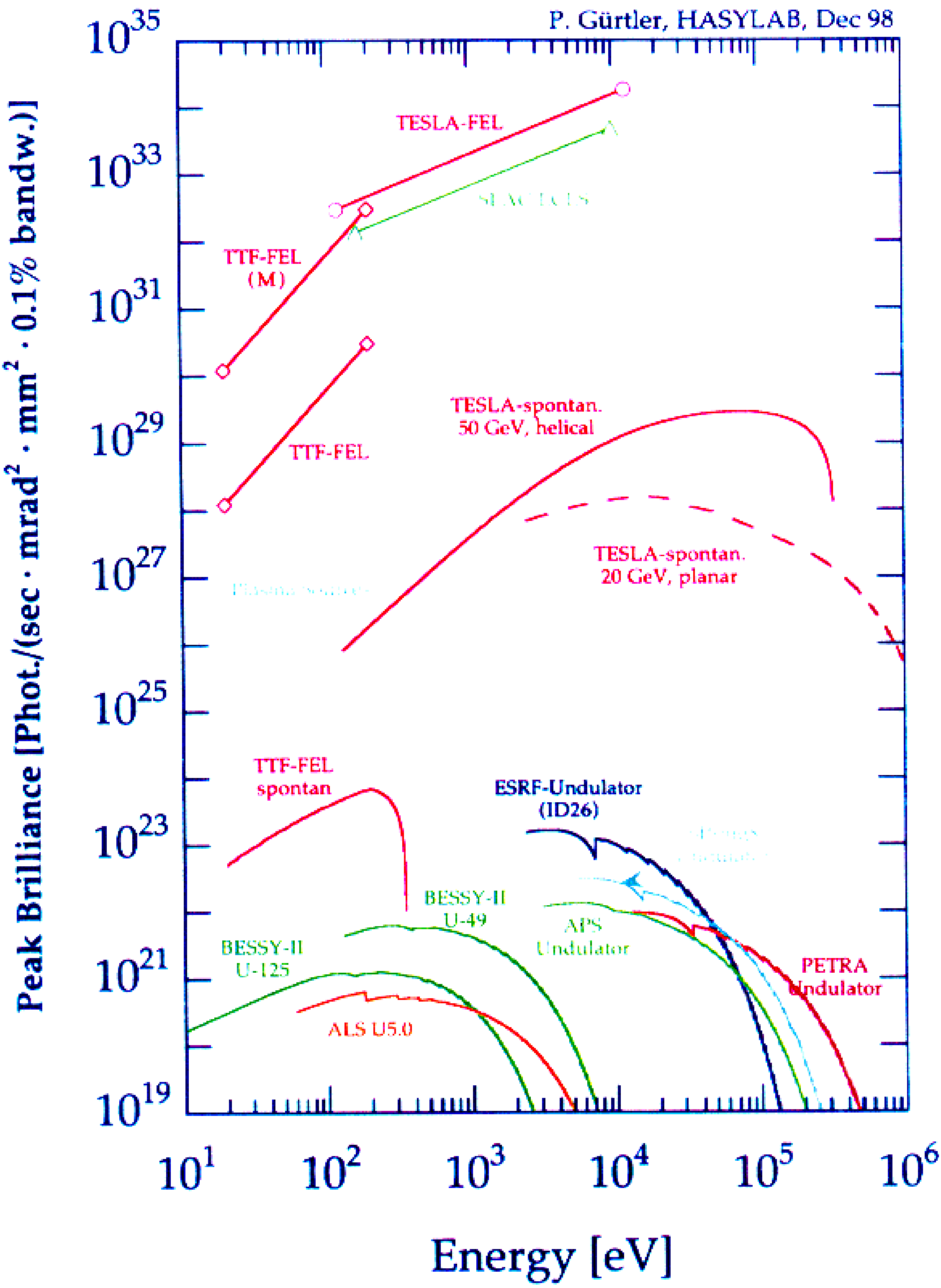




Spectral Brilliance (SB):

partially coherent source : $SB = \dfrac{spectral\ \ Flux}{4\pi^2 \Sigma_x \Sigma_{x'} \Sigma_z \Sigma_{z'}}$ $\quad\Big|\quad$ $\Sigma = \sqrt{\sigma_e^2 + \sigma_p^2}$

fully coherent source : $SB = \dfrac{spectral\ \ Flux}{(\lambda / 2)^2}$ $\quad\Big|\quad$ $\Sigma' = \sqrt{\sigma_e'^2 + \sigma_p'^2}$



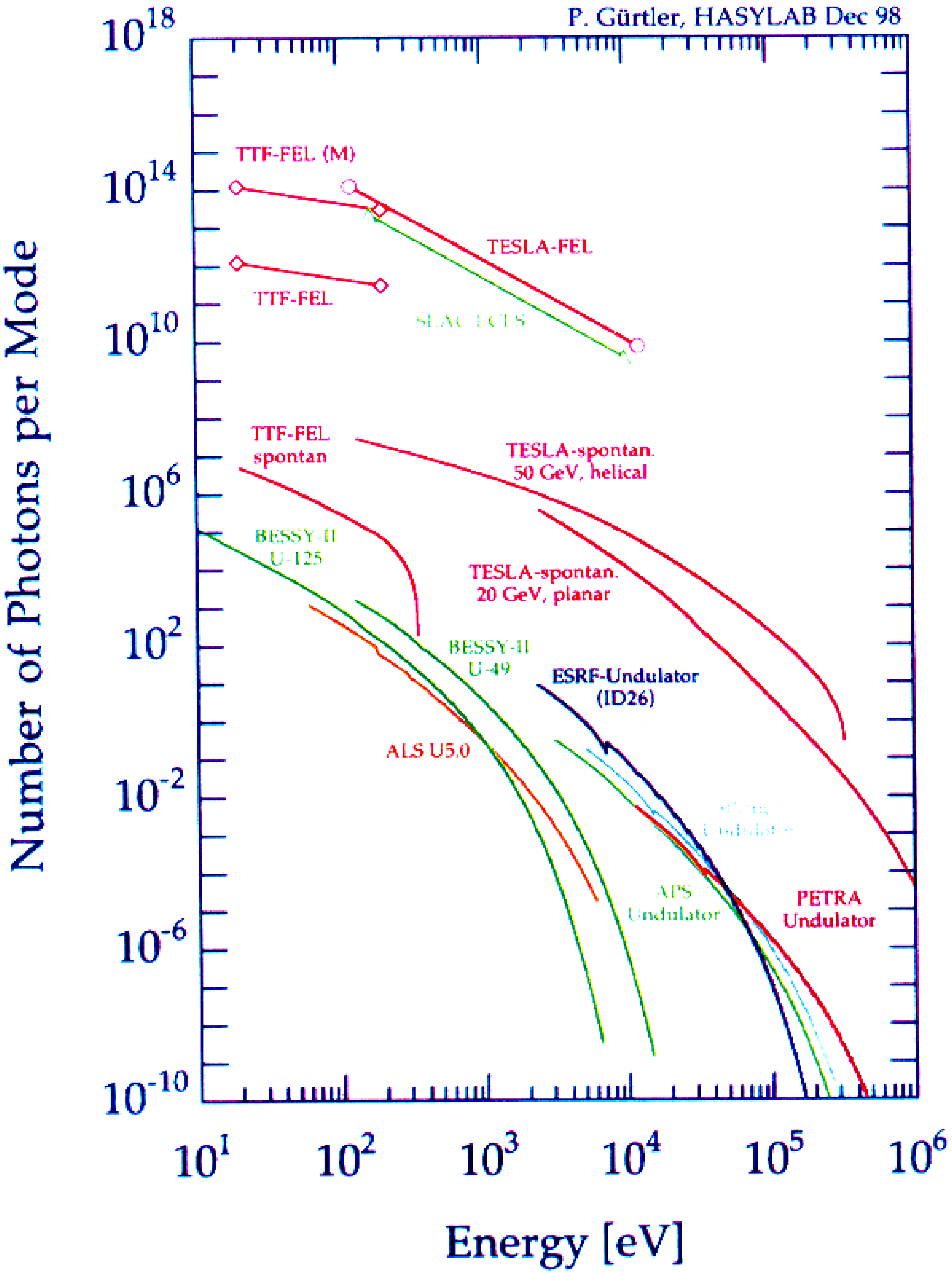
Spectral Brilliance (SB):

partially coherent source : $$SB = \frac{spectral\ Flux}{4\pi^2 \Sigma_x \Sigma_{x'} \Sigma_z \Sigma_{z'}}$$

fully coherent source : $$SB = \frac{spectral\ Flux}{(\lambda/2)^2}$$

$$\Sigma = \sqrt{\sigma_e^2 + \sigma_p^2}$$

$$\Sigma' = \sqrt{\sigma_e'^2 + \sigma_p'^2}$$



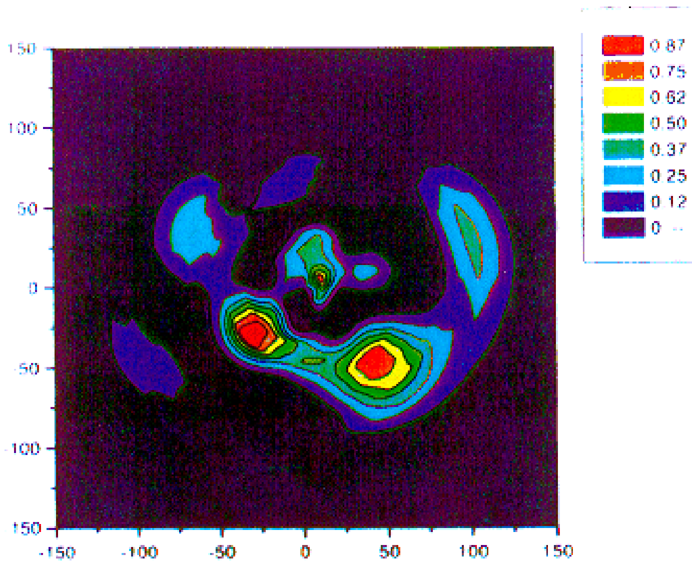
Number of Photons per Mode N :

$$N \equiv \frac{Peak\ \ Brilliance \cdot \lambda_{ph}^{3}}{4 \cdot c} \equiv$$ *average # photons which can interfere being in one quantum state ≡ "mode"*

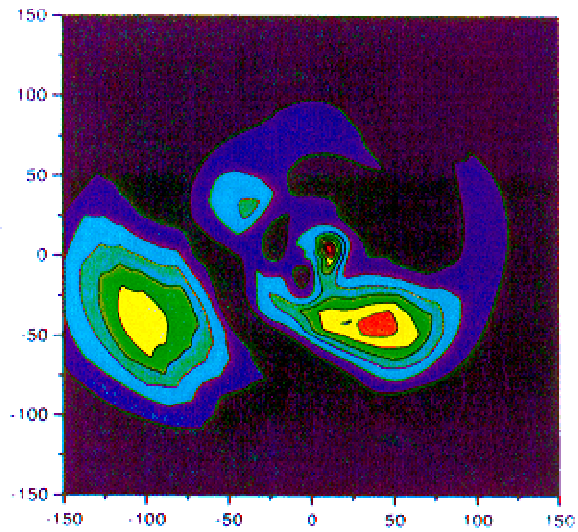
(Gaussian beam, not FT - limited)

Saldin, Schneidmiller & Yurkov (199

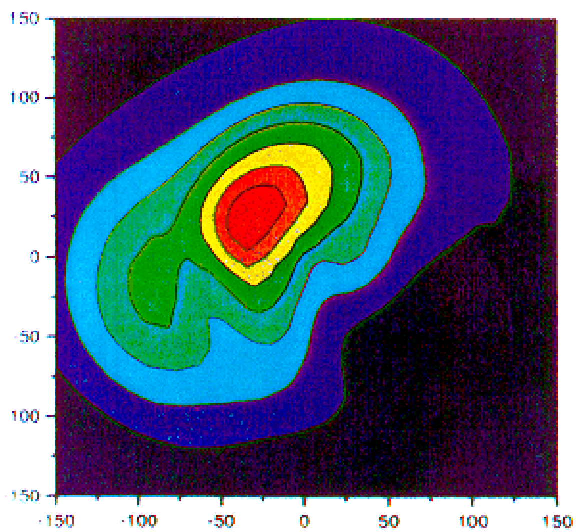
Power density, $\lambda = 70$ nm



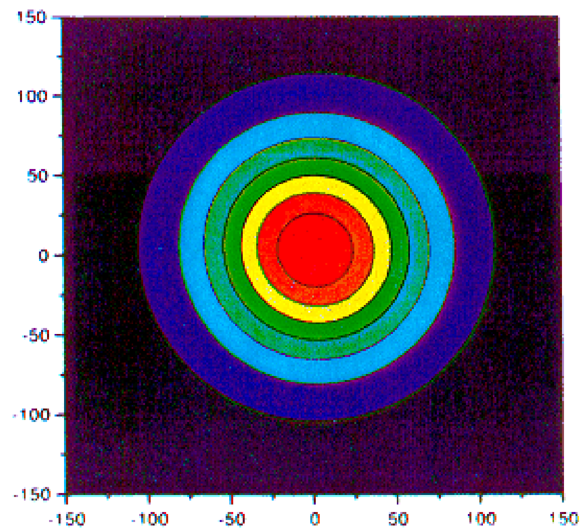
after 10 periods



the middle of the 1st module



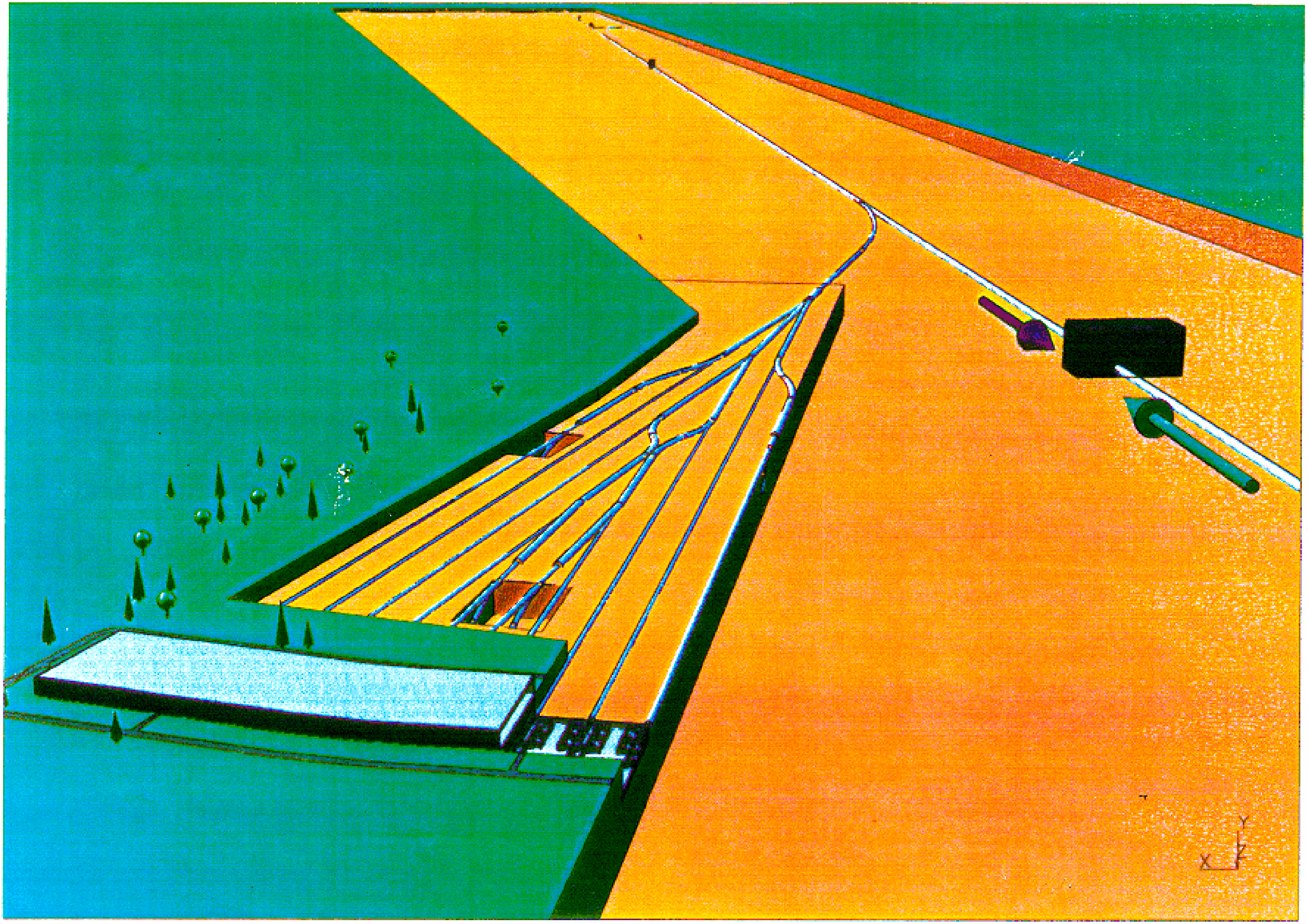
the end of the 1st module



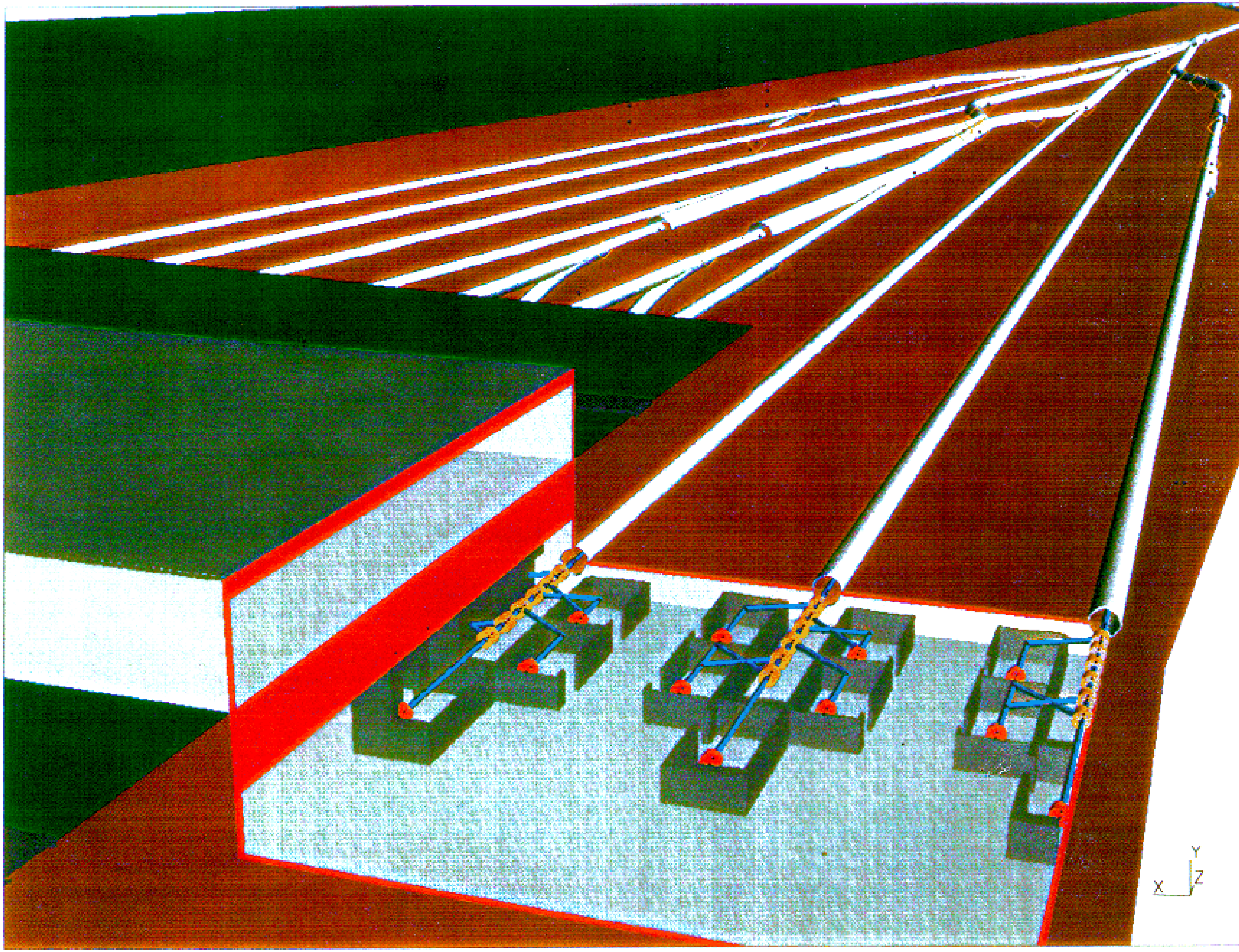
the end of the 2nd module

But: How many stations?

How many users?



HAHN@HASYHAHN, JUL31/14:02



HAHN@HASYCAD1 APR18/13:34

In a scientific case there always are:

- the "trivial" extensions (to do what we already can do now — "only" better)
  - smaller samples → lower quality required
    - → less time needed for crystal growth
    - → from 3D → 2D
    - → less replica required
  - + higher pressure
  - + better parameter control
  - higher element sensitivity { now Si sa... $< 10^9$ at/c... ↓ 10^4 ?
    - ↳ valence
  - better $\Delta E/E$ resolution
- and there are
  - the wild dreams
  - the unexpected surprises

But what about precise estimates??

e.g. scientific case for ESRF

- muscles
- liquid surfaces
- nuclear resonance
- inelastic scattering
  - ↳ new applications

}

- time resolution
- coherent imaging
- speckle
- magnetic spect...

XFEL -> sensitivity to impurities

Fig. 24:
Equation of state of ice VII obtained using a focused undulator beam. The different symbols correspond to different sets of measurements using diamond-anvil cells. The ice VII lattice is body-centred cubic, a typical spectrum is shown in the insert.

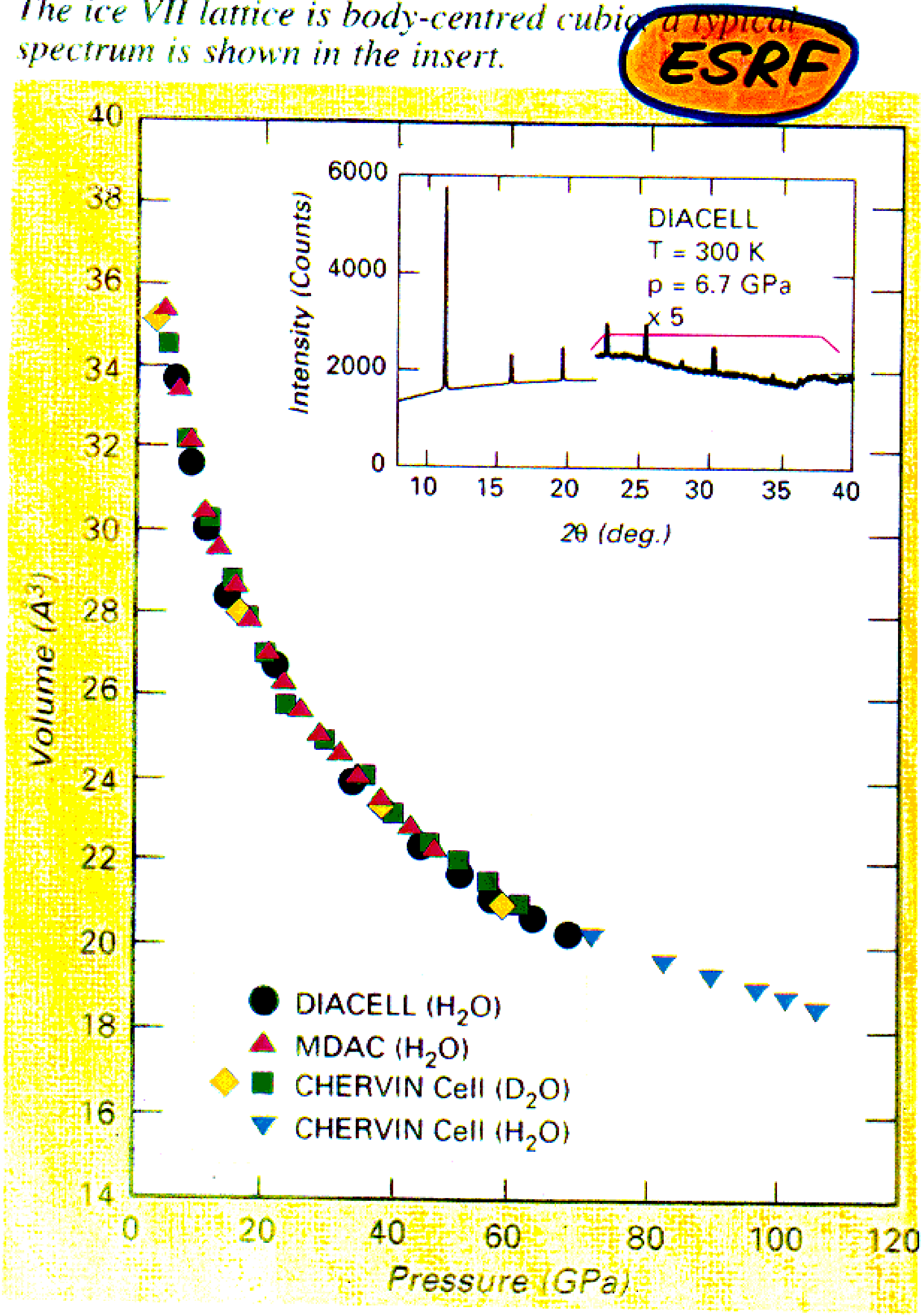
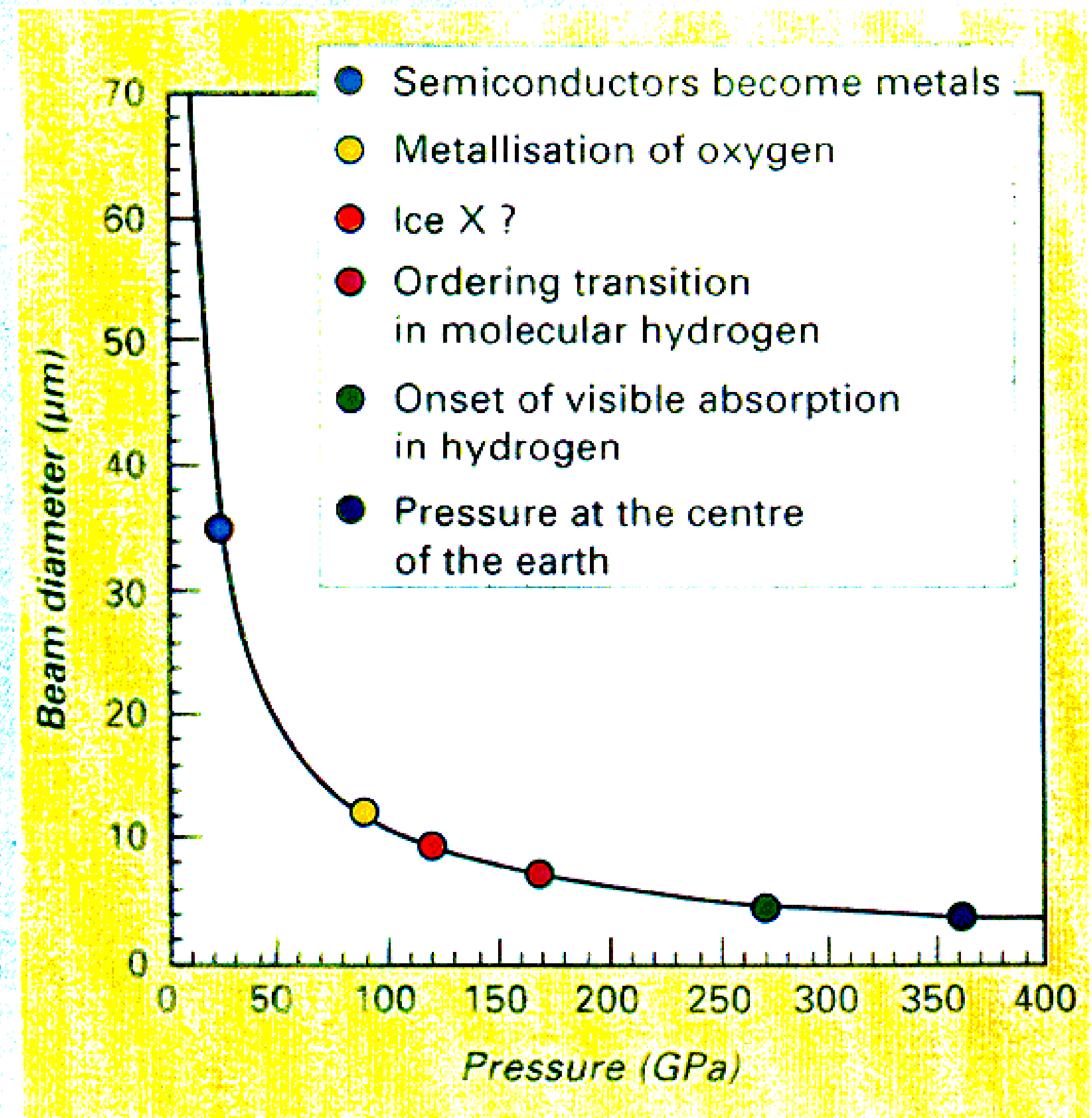


Fig. 20:
X-ray beam diameter necessary as a function of pressure to study various physical phenomena.



1 GPa = 10 kbar

ESRF (95)

Workshops on X-FEL Scientific Case

① W. Spicer, J. Arthur and H. Winick, October 1992, SLAC
20 - 2000 Å

② J. Arthur, G. Materlik and H. Winick, February 1994, SLAC
1 - 10 Å

③ T. Möller and B. Sonntag, November 1994 and April 1995, DESY
600 - 15 Å

④ 4th Generation Light Sources, January 1996, ESRF
ICFA meeting
J. Als-Nielsen for Scientifc Case

⑤ ~~This meeting~~ Febr. 1996, HASYLAB/DESY, Hamburg

⑥ Coherent Light Sources and Applications, Feburary/March 1996, KEK

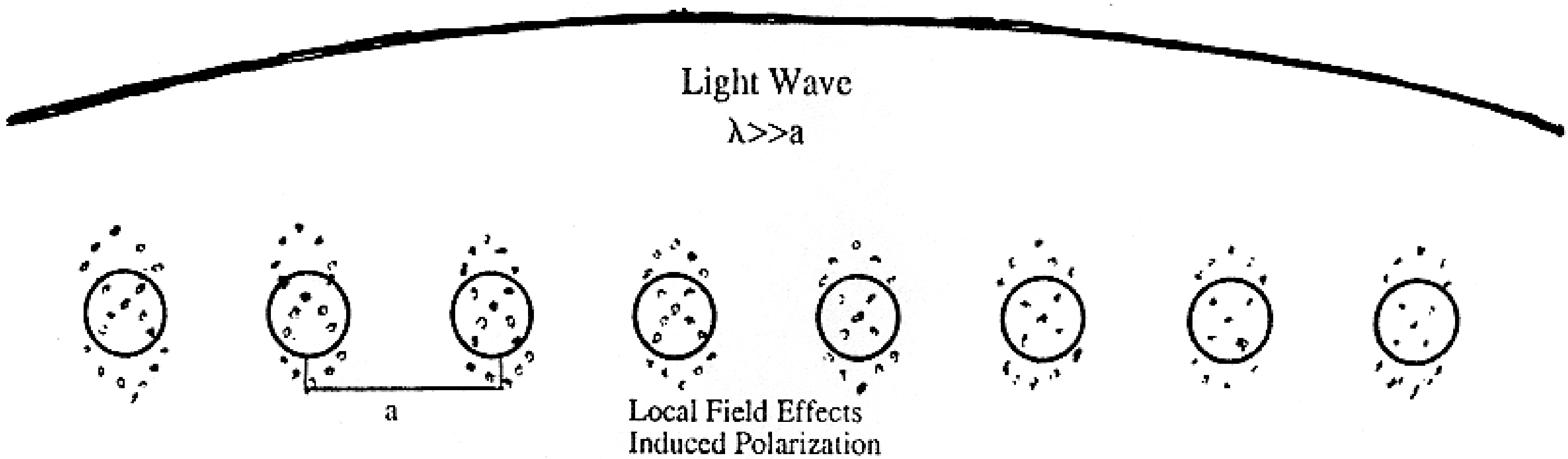
⑦ International Workshop on Scientific Applications of an X-FEL,
September 16./17, 1996, DESY

⑧ APS, Argonne, Spring 1997, planned

⑨ SLAC/SSRL Jan. 99

P. Eisenberger

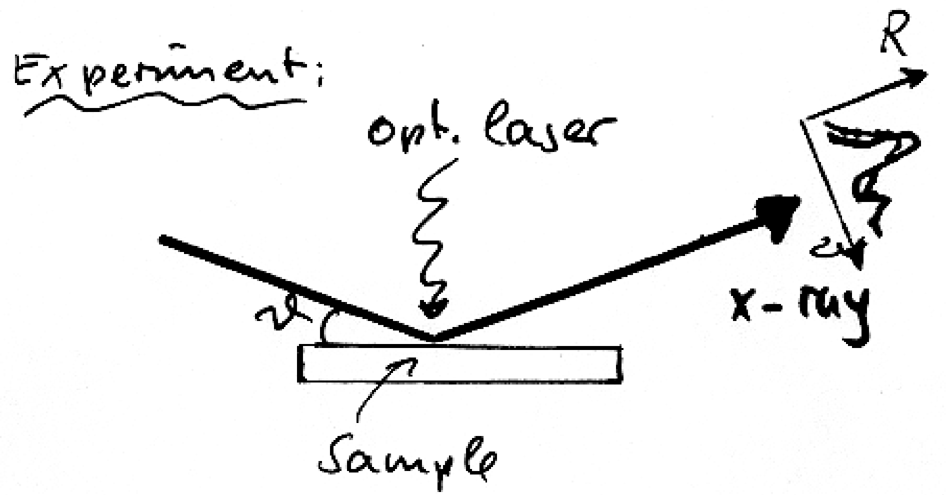
Non-Linear X-ray Phenomena
Light X-ray Mixing



$\bar{k}_{in} - \bar{k}_{out} = \bar{G} \pm \bar{q}_L$
$\omega_{in} - \omega_{out} = \pm \omega_L$

By doing crystallography on phase matched component
- local induced polarization can be determined

Can Extend to study various non-linear phenomena
- second harmonic
- stimulated Raman (Opt. Phonon)
- stimulated Brillouin (acoustic Phonon)



General Conclusion

P. Eisenberger

- The microscopic aspects of the interaction of light with crystals can be readily studied

  - Both linear optical and non-linear optical phenomena with XFEL

  - Includes polariton effects & exciton effects (magnons)

  - Only linear at ESRF & Argonne (even that limited)
    + small values of S cannot be explored
    + only crystals with relatively small x-ray absorption

Other Interesting Possibilites

- Time dependence

  - By delaying X-ray pulse relative to optical pulse can probe local relaxation phenomena

  - Can study development of gain (crystal in a cavity)

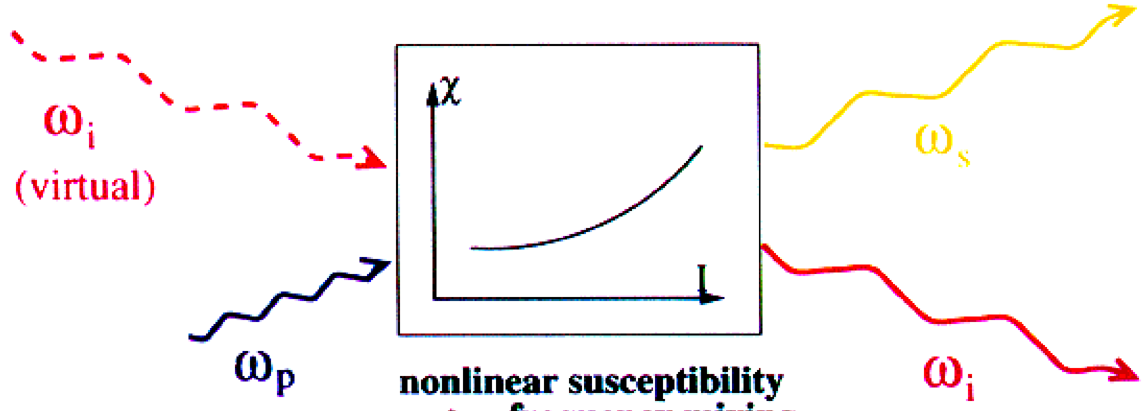
- Energy Transfer

  - With two light beams can simultaneously measure incident light fields effects and non-linear signal effects

- Produce Femtosecond X-ray beams
  - Use Femtosecond laser (higher LPL_p possible)

- Other modulations
  - acoustic waves, electron waves etc.

Parametric Down Conversion of X-Rays

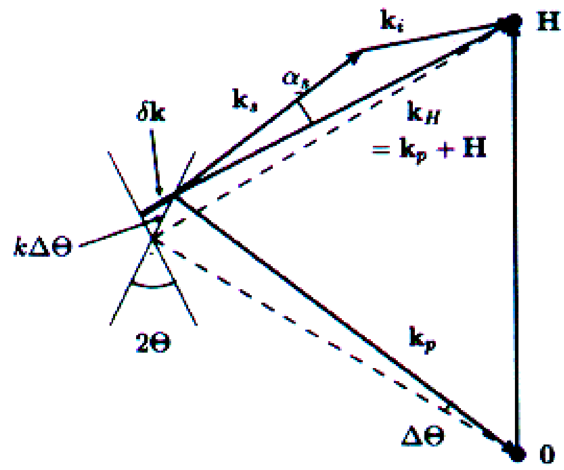


Here: Spontaneous decay: $\hbar\omega_p = \hbar\omega_s + \hbar\omega_i$

Real photon & vacuum fluctuation mix → 2 real photons

Phase matching condition:

$\mathbf{k}_p + \mathbf{H} = \mathbf{k}_s + \mathbf{k}_i$

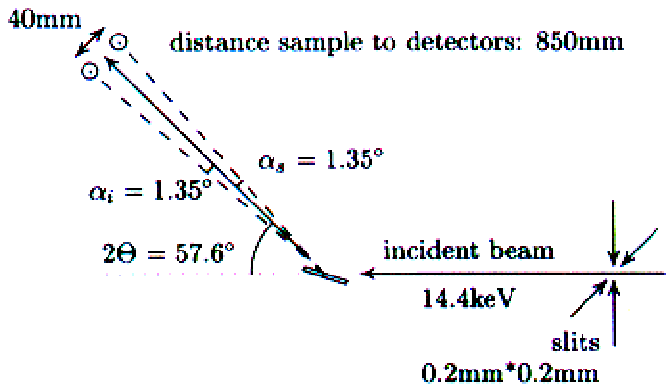


Possible applications:

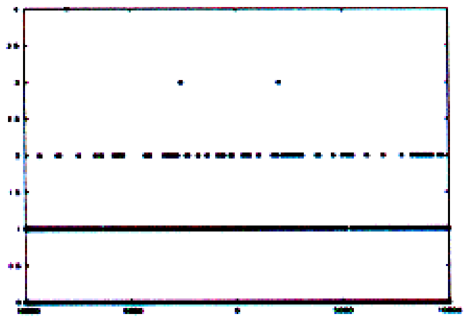
- Sub-Poisson statistics: Reduced radiation dose
- Two-photon interferometry
- Tests of the quantum theory (EPR, teleportation)

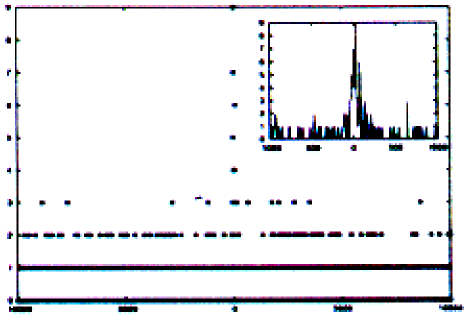
Experiment

The scattering geometry:



Time correlation spectra [3] show coincidence at 0 time difference above statistical background.

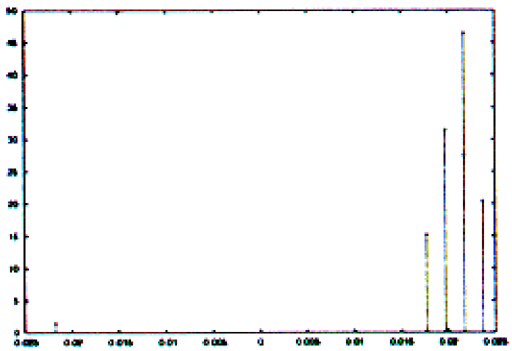




$-10\mu s$ Δt $+10\mu s$ $-10\mu s$ Δt $+10\mu s$

not fulfilled phase matching fulfilled

events:



$\Delta\Theta$

countrate now $\sim 1 \frac{\text{phot}}{\text{Min}}$

[1] P. Eisenberger, S.L. McCall, Phys. Rev. Lett. **26**, 684 (1971)
[2] Y.Yoda et al., J. Synchrotron Rad. **5**, 980 (1998)
[3] B. Adams et al., submitted to J. Synchrotron Rad.

Multi-photon K-shell absorption

With all 5.10^{12} photons/bunch focussed into 1μm diameter, ca. 10-100 photons/ atom are absorbed.

short K-shell lifetime (<1fs) => ~0.05 photons absorbed per atom per lifetime
(A. Kodre)

However, if radiation is not uniform within bunch, absorption rate increases

Also, if (D. Bilderback), capillary or Snigirev lens focussing to ca. 400Å diameter, ~100 photons absorbed per lifetime!

Thus, multiphoton X-ray absorption is feasible with XFEL

new area of X-ray physics
test theories of core-hole screening

Focussing with glass capillaries

Assumptions:

$\lambda = 1\,\text{Å}$, $1\,\mu$rad divergence, $100\,\mu m$ beam size
Glass capillary: Length 0.5-1 m, nearly perfect

Intensity increase in each dimension:

$$M = \frac{\text{critical angle}}{\text{divergence}} = \frac{2.6\,\text{mr}}{0.001\,\text{mr}} = 2\,600$$

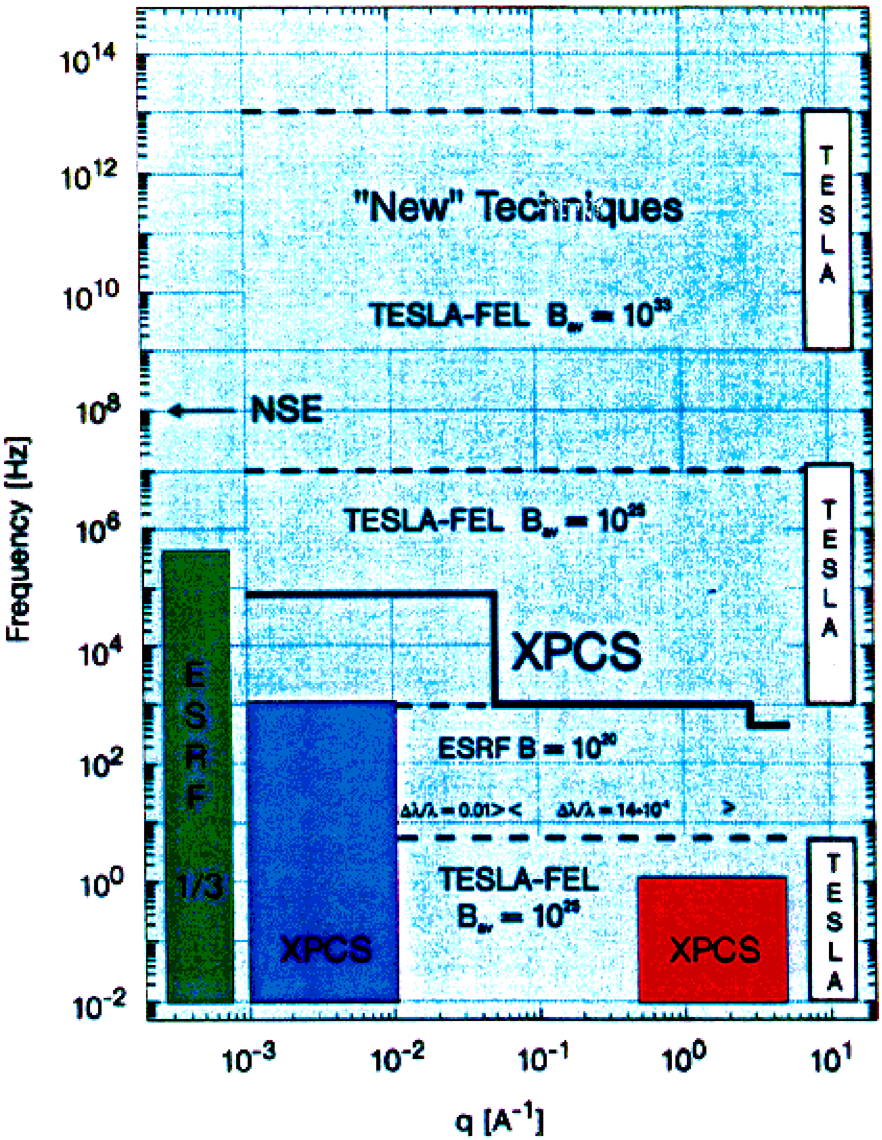
$\Rightarrow$ beam can be squeezed by $\frac{1}{2600}$ to 380 Å

Intensity gain:

$M^2 \cdot \text{efficiency} = 2600^2 \cdot 0.5 = 3.4 \cdot 10^6$

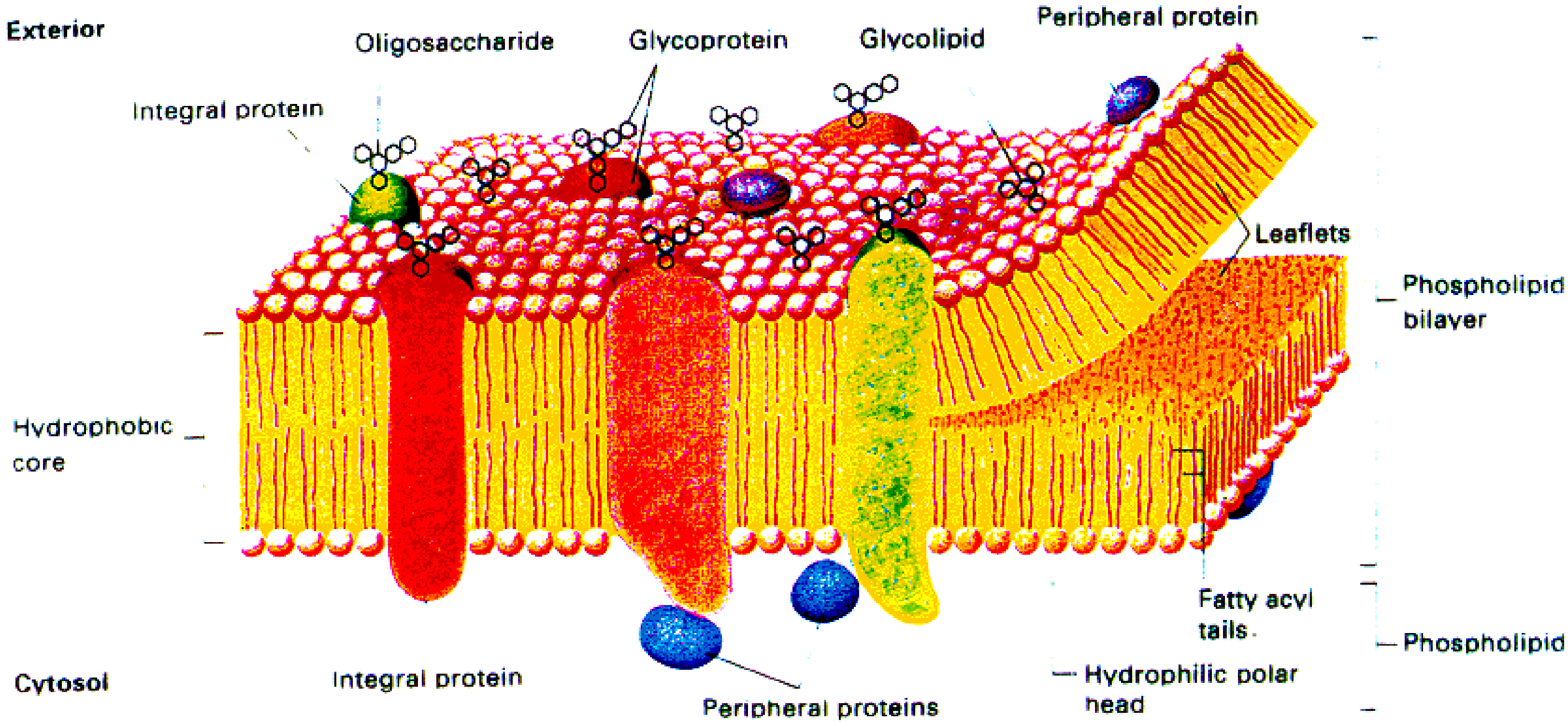
(D. Bilderback)

X-ray Photon Correlation Spectroscopy



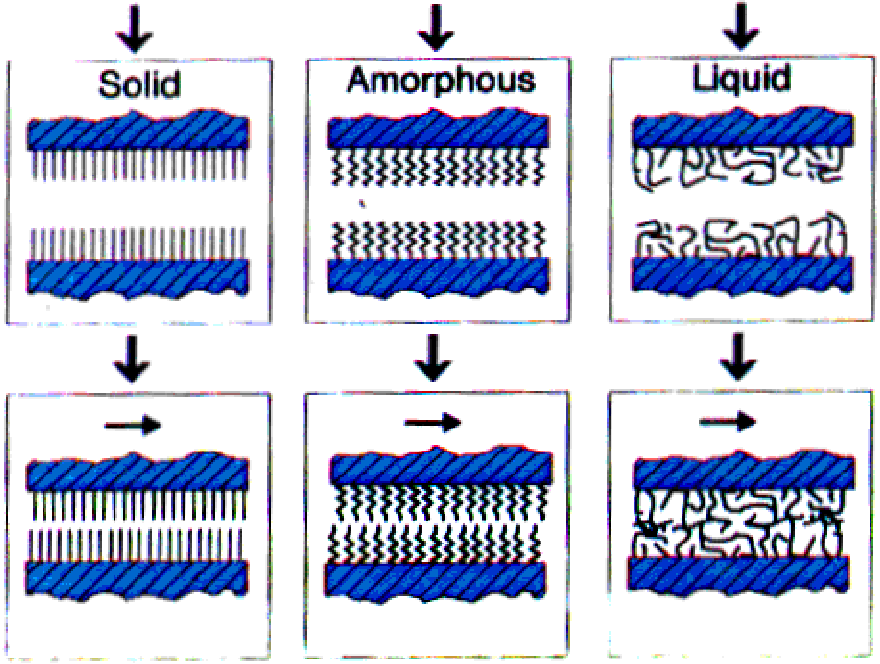
Frequency-wavevector ranges accessible to XPCS and new (puse-probe, stroboscopic) techniques. The [redacted] shaded areas indicate the frequency-q range where XPCS experiments have already been performed. The horizontal line indicates the ranges which are accessible to XPCS assuming a brilliance $B = 10^{20}$ and 2D detection. With increasing q-vector larger longitudinal coherence lengths have to be used requiring higher monocromaticity at the expense of flux. The vertical bars indicate the accessible frequency ranges defined by either the repetition rate of the TESLA source or the pulse length.

Structural biology: membranes



▲ **Figure 13-1** A phospholipid bilayer constitutes the basic structure of biological membranes. The hydrophobic fatty acyl tails of the phospholipids form the middle of the bilayer; the polar, hydrophilic heads of the phospholipids line both surfaces. Integral proteins have one or more regions embedded in the lipid bilayer. Peripheral proteins are primarily associated with the membrane by specific protein-protein interactions. Oligosaccharides bind mainly to membrane proteins; however, some bind to lipids, forming glycolipids.

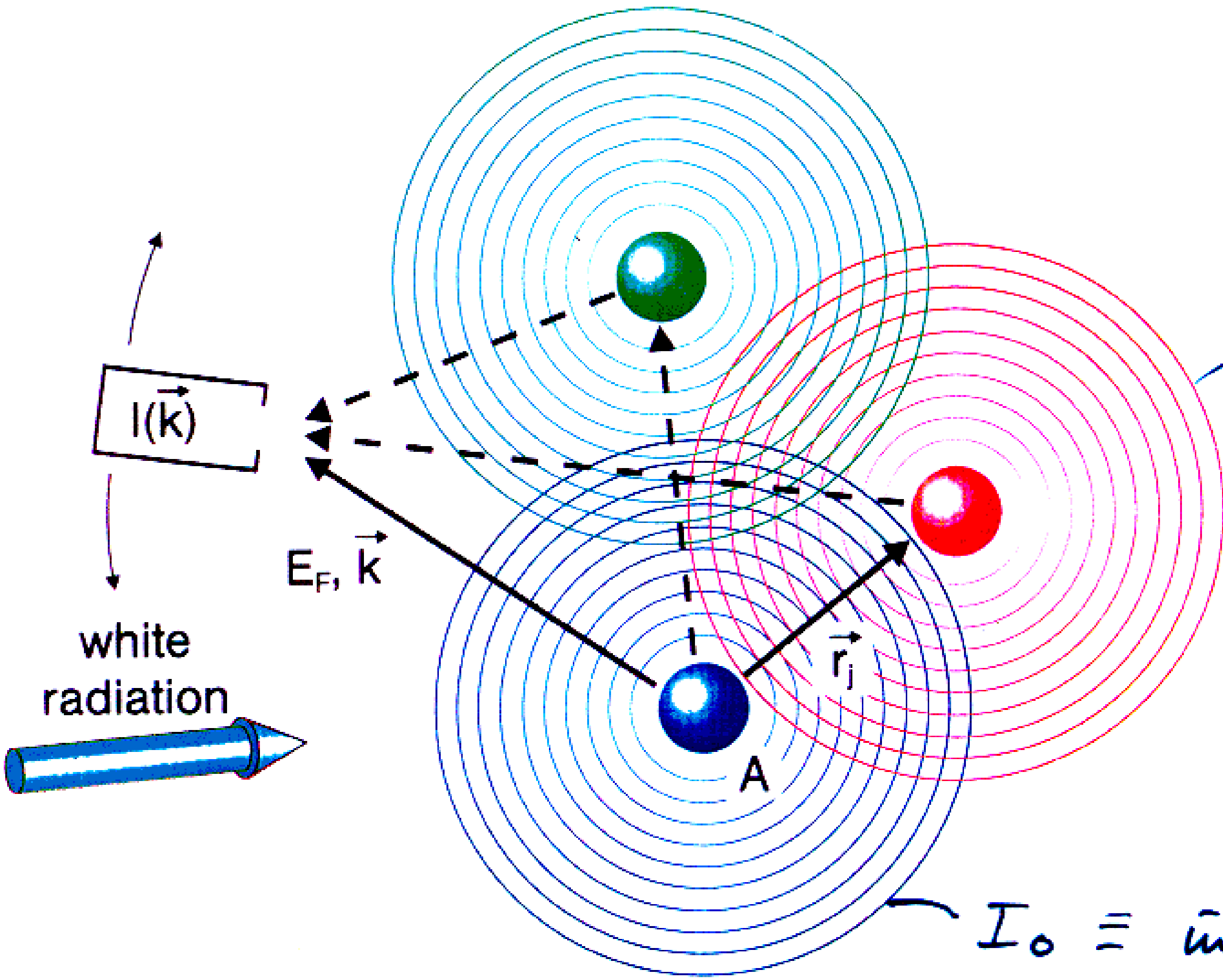
3-dimensional → 2-dimensional → clusters →



Interfaces during friction. Depending on pressure and velocity different phases may occur

Occurence of slip-stick motion

A. Szöke (1986)



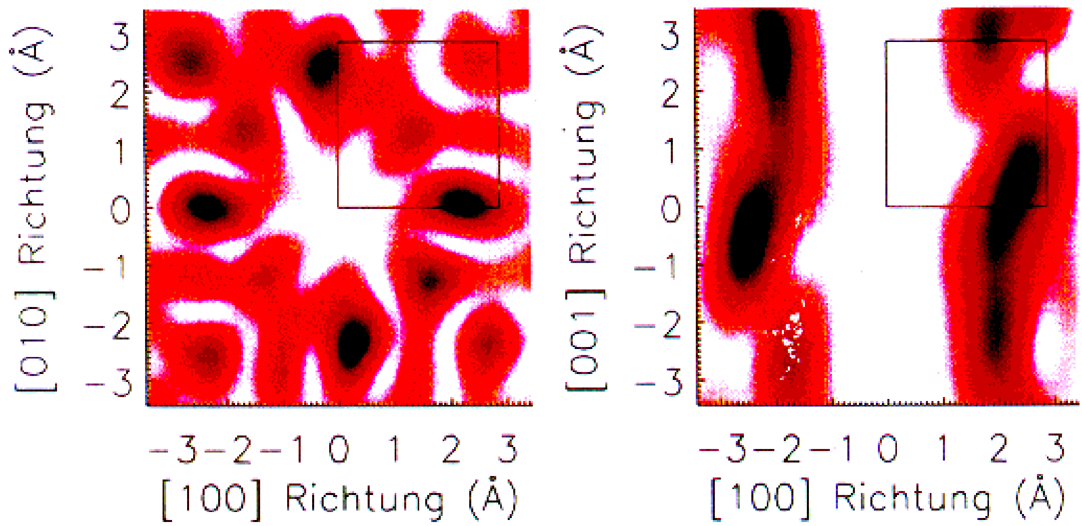
$a_j \equiv$ wave amplit scattere by j-at

$I_0 \equiv$ intensity of source atom

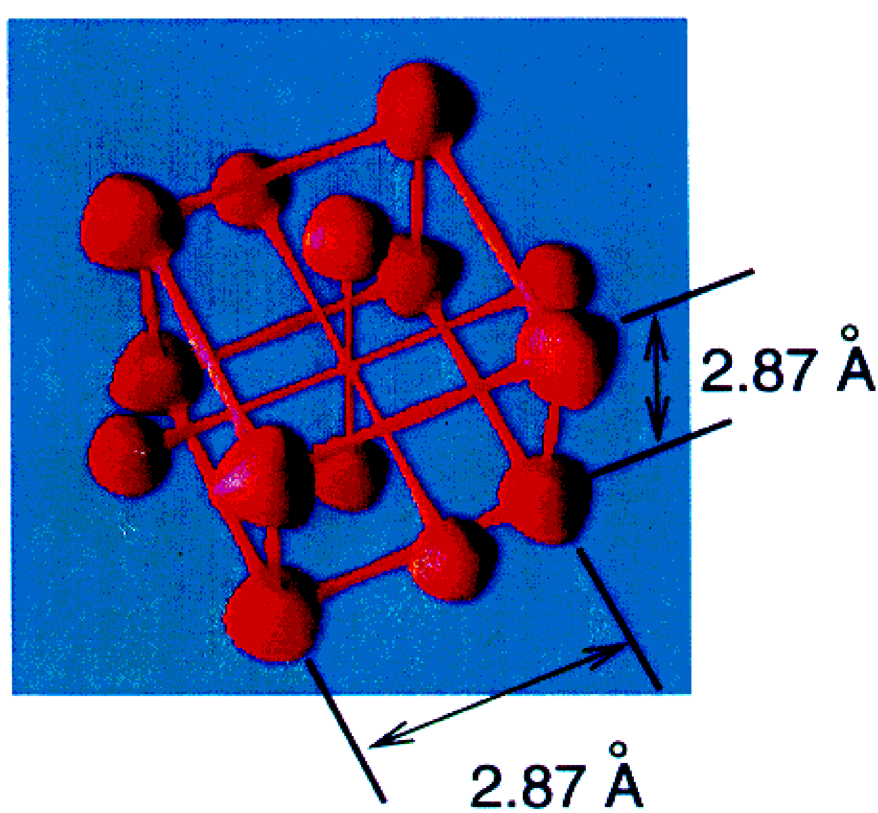
$$I = I_0/R^2 \left[1 + \left|\sum a_j\right|^2 + 2\,\mathrm{Re}\left(\sum a_j\right) \right]$$

Rekonstruktionen von Fe

2-dimensionale Rekonstruktionen



3-dimensionale Rekonstruktion



T. Hiort, E. Kossel, D. V. Novikov, B. Adams, Y. Nishino, G. Materlik

Mößbauer Spectroscopy

New nuclei:

e.g. ^{45}Sc at 12.4 KeV

extremely narrow resonance

$$\Gamma / E_0 = 1.2 * 10^{-19}$$

$\Longrightarrow$ energy of photon is shifted over full Γ within 1 mm of the gravitational field

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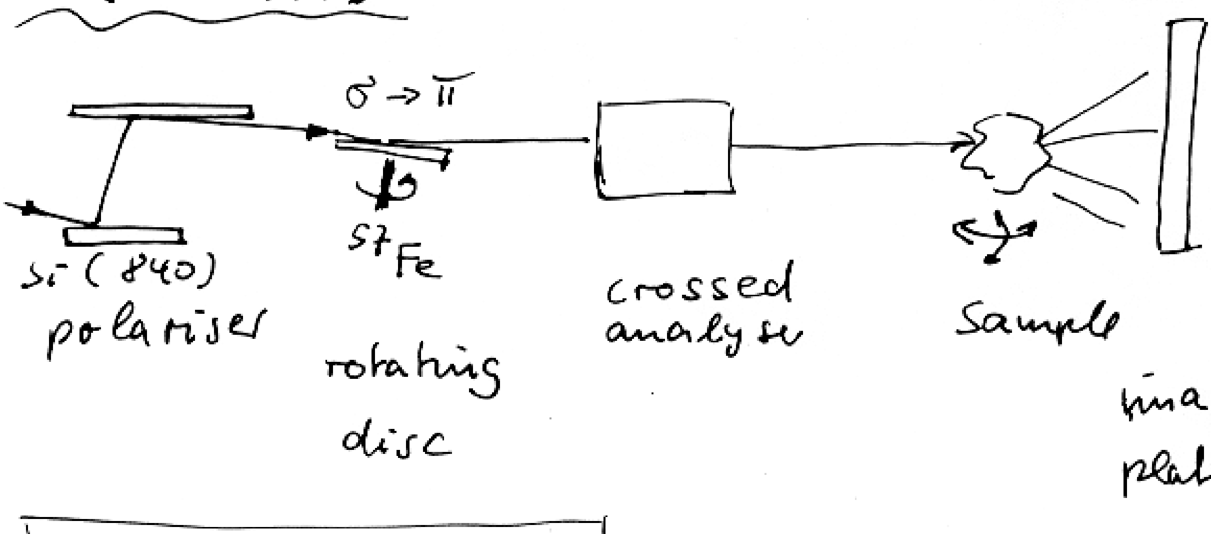
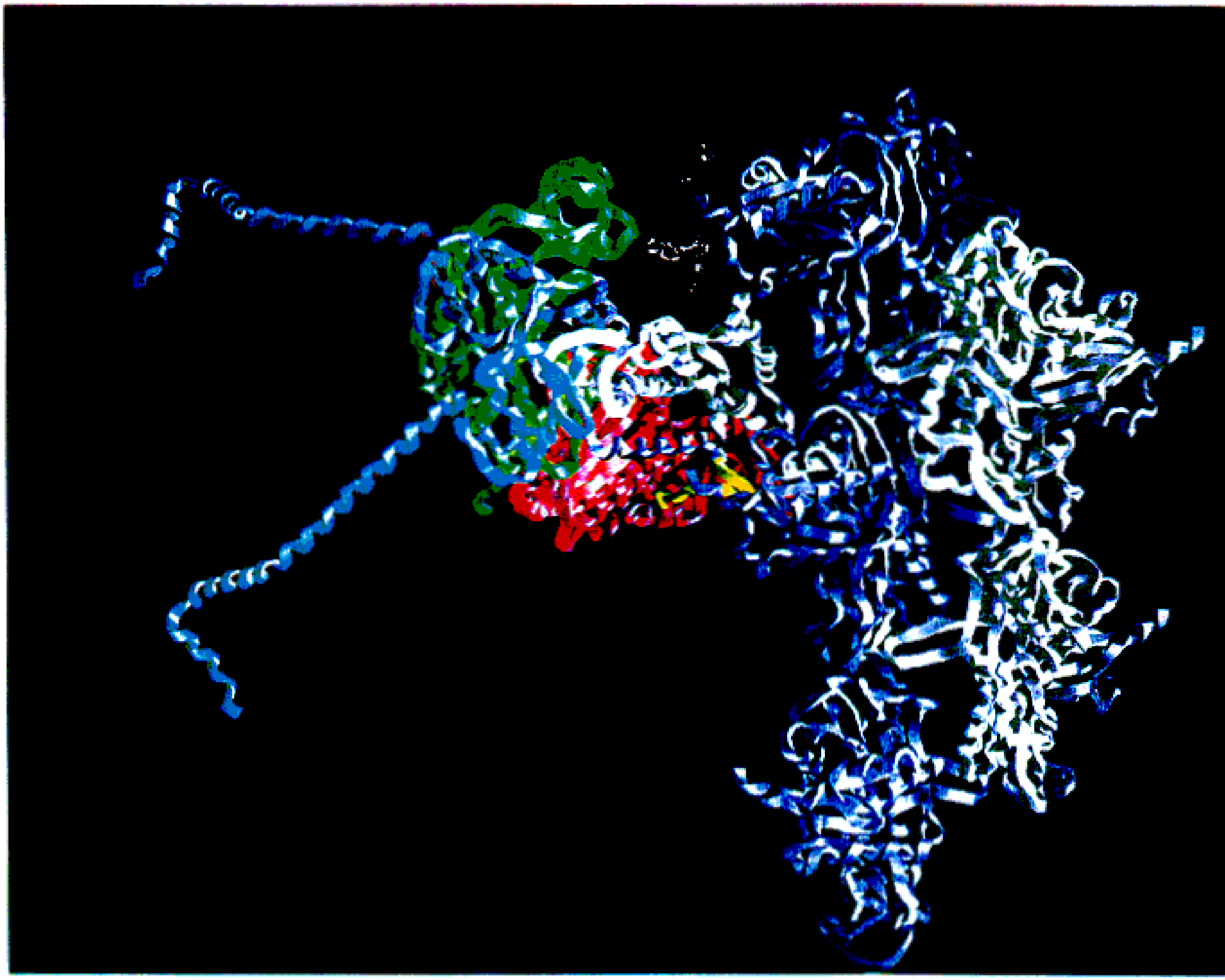
NR - MAD



$$\boxed{f'_{^{57}Fe} \sim 500\, e^-}$$

1 Fe-atom / subunit

could perhaps solve the Ribosome structure



myosin filament

lever arm flips in m seconds

myosin head

motor of movement

actin - filament