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UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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UNITED NATIONS INDUSTRIAL DEVELOPMENT ORGANIZATION

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SECOND SCHOOL ON THE USE OF SYNCHROTRON RADIATION IN SCIENCE AND TECHNOLOGY:
"JOHN FUGGLE MEMORIAL"

25 October - 19 November 1993

Miramare - Trieste, Italy

Crystal Monochromators

S. Bernstorff
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Italy

2. School on the Use of Synchrotron Radiation in Science and Technology

Miramare (Trieste)
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Crystal Monochromators

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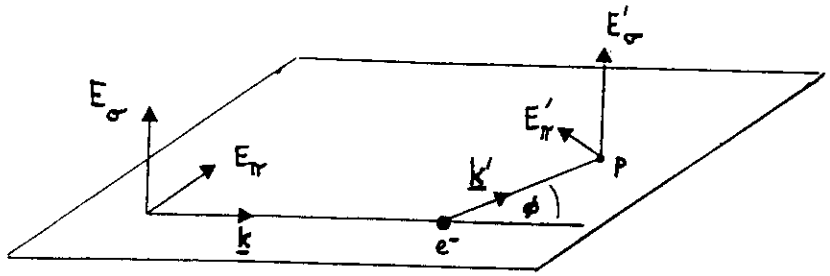
2. Introduction into the elementary theory of elastic X-ray Scattering

2.1 Scattering at a free electron



Let us assume that an electro-magnetic wave having an electrical field $\underline{E}_0 \exp[i(\omega t - \underline{k}\cdot\underline{x})]$ impinges onto an electron. The electric field induces oscillations of the electron charge and thus an oscillating dipole of size:

$$\underline{M} = -(e^2/ m\omega^2)\, \underline{E}_0 \exp(i\omega t) \qquad (1)$$

This oscillating dipole emits now also a wave. This wave has a wave vector $\underline{k}'$ (with $|\underline{k}'| = |\underline{k}|$), and its electrical field - in a sufficiently large distance $\underline{r}_p$ from the dipole - is given by (see Jackson):

$$\underline{E}_p = -(e^2/mc^2)(1/r_p)(\underline{n}' \times \underline{E}_0) \times \underline{n}' \exp[i(\omega t - \underline{k}'\cdot\underline{r}_p)] \qquad (2)$$

where $\underline{n}'$ is the unit vector in $\underline{k}'$ direction and $r_0 = e^2/mc^2$ = 2.818 (exp -15) m is the classical electron radius.

In the case of σ polarisation we have

$$E_\sigma' = -E_\sigma(e^2/mc^2)(1/r_p) \exp[i(\omega t - \underline{k}'\cdot\underline{r}_p)] \qquad (3)$$

while for the case of π polarisation we get

$$E_\pi' = -E_\pi(e^2/mc^2)(1/r_p) \exp[i(\omega t - \underline{k}'\cdot\underline{r}_p)] \cos\phi \qquad (4)$$

where ϕ is the scattering angle.

This last case shows the possibility to use scattering in order to linearly polarise a beam which previously was not polarised. Indeed, for $\phi = 90°$ only the σ component will be scattered.

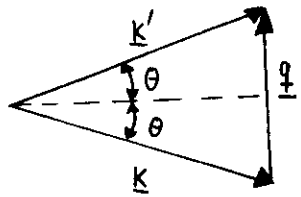
2.2 Scattering by an atom; the Atomic Scattering Factor

The scattering amplitude for a collection of electrons in an atom is the sum of the scattering amplitudes of all electrons taking into account the phase difference arising from the spatial distribution of the electrons which are assumed to be free.
This assumption is true for photon energies much higher than the binding energy of the innermost shell (for lower photon energies the bound character of the atomic electrons would become noticeable).
Let us now consider a X-ray beam which impinges onto an atom whose n electrons have the position vectors $\underline{r}_n$. For simplicity let us use σ polarisation. Then, in a point P in a sufficiently large distance, the scattered wave is given by the sum of all the n terms of type (3) created by n single atoms:

$$E_p = -E_0(e^2/mc^2) \sum_{n=1}^{Z} 1/(|\underline{r}_p-\underline{r}_n|)\ \exp[-i\underline{k}'\cdot(\underline{r}_p-\underline{r}_n)]\ \exp[-i\underline{k}\,\underline{r}_n]$$

$$= -E_0(e^2/mc^2)\ (1/r_p)\ \exp[-i\underline{k}'\cdot\underline{r}_p] \sum_{n=1}^{Z} \exp[-i\underline{r}_n\underline{q}] \qquad (5)$$

with $\underline{q} = \underline{k}' - \underline{k}$ = scattering vector and Z=atomic number.



Now we pass to the more realistic case in which each electronic state "i" has a continuos electron density ($\rho_i(\underline{r})$) distribution. Then, summing over all states "i" and integrating over all volume elements dv, equation (5) can be written as:

$$E_p = -E_0(e^2/mc^2)(1/r_p)\ \exp[-i\underline{k}'\cdot\underline{r}_p] \sum_i \int_V \rho_i(\underline{r})\ \exp[-i\underline{r}\,\underline{q}]\ dv \qquad (6)$$

The last part of equation (6) is called Atomic Scattering Factor or Form Factor:

$$f = \sum_i f_i = \sum_i \int_V \rho_i(\underline{r})\ \exp[-i\underline{r}\,\underline{q}]\ dv \qquad (7)$$

Thus the intensity scattered by an atom is given by:

$$I_p = I_0\ (e^2/mc^2)^2\ (1/r_p)^2\ f^2 \qquad (8)$$

f is therefore the relation between the intensities which are elastically scattered by an atom and by an classical electron.

If the $\rho_i(\underline{r})$ have spherical symmetries, then f can be written as:

$$f = \sum_i \int_0^\infty 4\pi\ r^2\ \rho_i(\underline{r})\ (\sin kr / kr)\ dv \qquad (9)$$

with $k = |\underline{q}| = 4\ \pi\ \sin\theta / \lambda$).

We note that in the case of $\underline{q} = 0$ (forward scattering)

$$f = Z \qquad (10)$$

Up to now we assumed that the photon energy E_{ph} would be much larger than the binding energies E_B of the atom. With this approximation effects of Anomalous Scattering are not taken into account. These effects however can be included if correction terms are added to f:

$$f = f_0 + f' + if'' \qquad (11)$$

where f_0 is the structure factor for $E_{ph} > E_B$

f' and f'' are real and imaginary part of the contribution due to the presence of a natural frequency ω' in the atom close to the frequency ω of the incoming photon beam.

It can be shown that f' and f'' are related by the Kramers-Kronig relationship

$$f'(\omega) = 2/\pi \int [(\omega' f''(\omega')) / (\omega^2 - \omega'^2)] \, d\omega'$$

Furthermore,

$$f''(\omega) = (m \omega / 4\pi e^2) (A/N) \mu(\omega) \qquad (12)$$

where N = Avogadro's number
A = atomic weight
$\mu(\omega)$ = linear absorption coefficient

2.3 Scattering from a crystal: the Structure Factor

We consider now an assembly of n atoms, each characterised by a Scattering Factor f_n. In the crystal lattice the atoms are defined by the unit vectors $\underline{a}_1$, $\underline{a}_2$, and $\underline{a}_3$. The dimensions of the crystal are given by N_1, N_2, and N_3. Then the position of the n^{th} atom in the m^{th} unit cell can be written as:

$$\underline{r}_{nm} = \underline{R}_m + \underline{r}'_n \qquad (13)$$

where

$$\underline{R}_m = m_1\underline{a}_1 + m_2\underline{a}_2 + m_3\underline{a}_3 \qquad (14)$$

defines the unit cell and $\underline{r}'_n$ the atom in it.

The electric field in a sufficient far away point P is given by:

$$E_p = -E_0(e^2/mc^2)(1/r_p) \exp[-i\underline{k}'\cdot\underline{r}_p] \times$$

$$\sum_n f_n \exp[-i\underline{r}_n' \underline{q}] \sum_m \exp[-i\underline{R}_m \underline{q}] \qquad (15)$$

The factor

$$\boxed{F_{\underline{q}} = \sum_n f_n \exp[-i\underline{r}_n' \underline{q}]} \qquad (16)$$

is called Structure Factor.

In eq. (15) the terms in the sum over the unit cells can be divided into three separate sums, using eq. (14). Then each sum has the following form:

$$\sum_{m_1=0}^{N_1-1} \exp[-i\underline{q}\, m_1\underline{a}_1] = (\exp[i\underline{q}\, N_1\underline{a}_1] - 1)/(\exp[i\underline{q}\, \underline{a}_1] - 1) \qquad (17)$$

The intensity is proportional to the product of the square brackets of each of these terms:

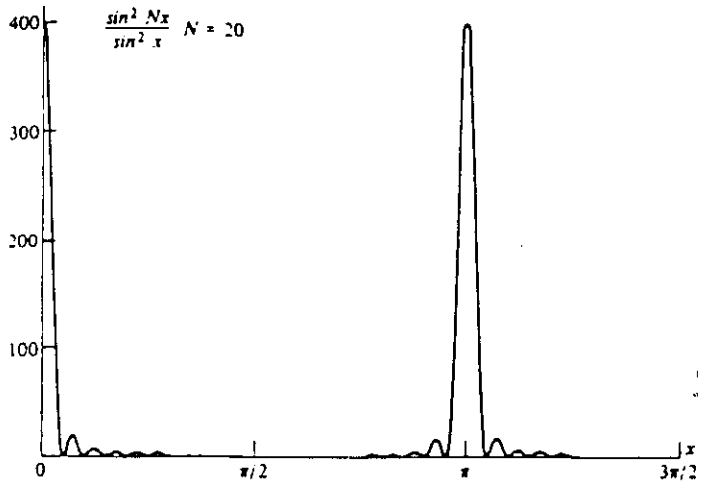
$$\{\sin^2 (1/2)\, \underline{q}\, N_1 \underline{a}_1\} \,/\, \{\sin^2 (1/2)\, \underline{q}\, \underline{a}_1\} \qquad (18)$$

This function has a maximum only for $\underline{q}\, \underline{a}_1 = 2\pi h$, where h is an integer.

Equivalent conditions are valid for the other sums; thus an diffraction peak can be obtained only if:

$$\begin{aligned} &\underline{q}\, \underline{a}1 = 2\pi\, h \\ &\underline{q}\, \underline{a}2 = 2\pi\, k \\ &\underline{q}\, \underline{a}3 = 2\pi\, l \quad \text{with h, k, l integers} \end{aligned} \qquad (19)$$

Note that the width of each peak is proportional to $1/N_1N_2N_3$, i.e. inverse proportional to the number of involved atoms.



The function $(\sin^2 Nx)/\sin^2 x$ for $N = 20$. The function peaks at values o x which are integral multiples of π, and it is essentially zero everywhere else.

The above equations can be rewritten using the vectors of the reciprocal lattice. If we define:

$$\underline{b}1 = 2\pi\, (\underline{a}2 \times \underline{a}3) \,/\, \{\underline{a}1\, (\underline{a}2 \times \underline{a}3)\} \qquad (20)$$

and the cyclic combinations to obtain $\underline{b}2$ and $\underline{b}3$, then

$$\underline{a}i\, \underline{b}j = 2\pi\, \delta ij \qquad (21)$$

These conditions are equivalent to

$$\underline{q} = \underline{H} \qquad (22)$$

with the vector $\underline{H}$ of the reciprocal lattice equal to

$$\underline{K} = h\, \underline{b}1 + k\, \underline{b}2 + l\, \underline{b}3 \qquad (23)$$

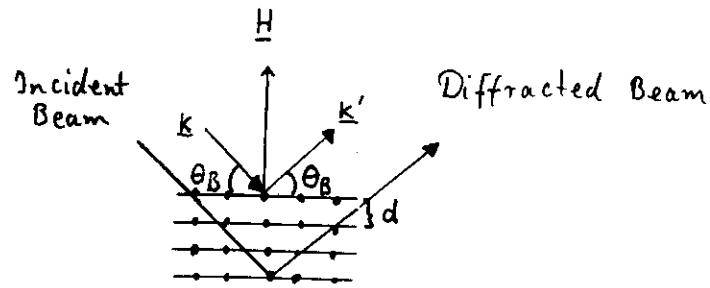
The condition (23) means that the scattering vector is equal to a vector of the reciprocal lattice.

We remember that

$$|\underline{H}| = 2\pi \,/\, d\{h,k,l\} \qquad (24)$$

Thus the relation (23) is equivalent to the well know Bragg's equation:

$$\boxed{2\, d\{h,k,l\} \sin \theta_B = n\, \lambda} \qquad (25)$$



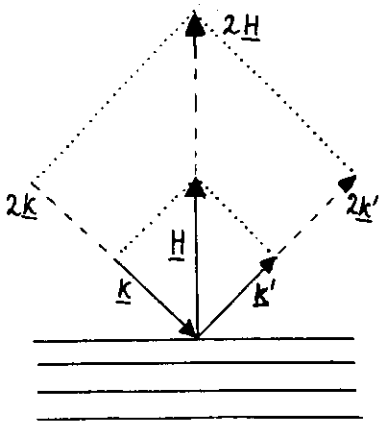
The Structure Factor

$$F_{\underline{H}} = \sum f_n \exp[-i\underline{r}_n \underline{H}]$$

determines if the diffraction on lattice planes, which are defined by $\underline{H}$, takes place or not.
For example, for the Zinc Blende structure the following rules for the components of $\underline{H}$ are valid:

for:	$h + k + l = 4n$	$F_{hkl}^2 = 16\,(f_A + f_B)^2$
	$h + k + l = 2(2n+1)$	$F_{hkl}^2 = 16\,(f_A - f_B)^2$
	h, k, l all odd	$F_{hkl}^2 = 16\,(f_A^2 + f_B^2)$
	h, k, l partly even, odd	$F_{hkl}^2 = 0$

For Si and Ge the same rules are valid with A = B. Using these rules it is possible to calculate which reflexes, and which harmonics of them, are allowed.



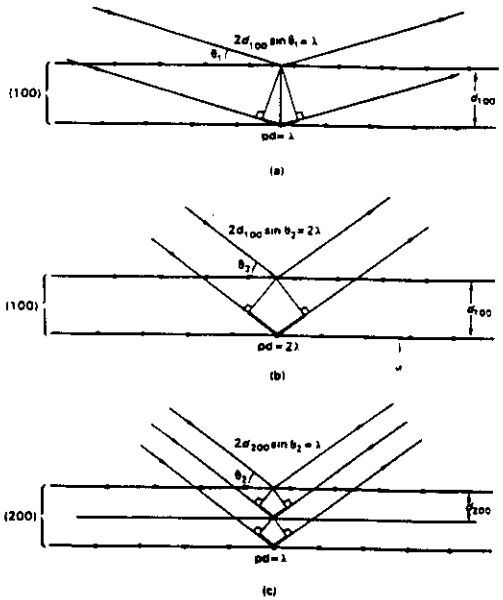


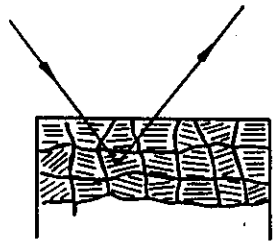
Fig. 3.7 Formation of (a) the first-order reflection from the (100) planes, (b) the second-order reflection from the (100) planes and (c) the first-order reflection from the (200) planes; pd = path difference. Note that (b) and (c) are ...

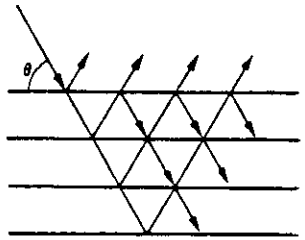
3. Short Introduction into the Dynamical Theory of X-ray Diffraction

The intensity and form of a diffracted X-ray beam depends on the quality of a single crystal. For a "perfect" crystal one has to take into account that a diffracted beam is again diffracted. The double diffracted beam has again the direction of the incident beam.

The Kinematical Diffraction Theory neglects this effect, while the Dynamical Diffraction Theory includes it.

Kinematical Theory	Dynamical Theory
- highly imperfect crystals	- highly perfect crystals
- mosaic crystals	- multiple scattering
- small crystals	- extinction



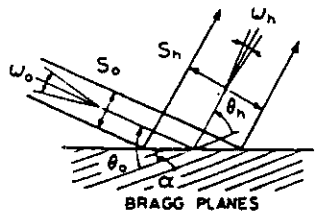


1914	Darwin	1. dynamical theory
1916/17	Ewald	independently developed theory; different, more sophisticated treatment of dynamical diffraction
1931	von Laue	Ewald's theory reformulated; problem now based on the solution of the Maxwell equations for a medium with a periodic complex dielectric constant; with period comparable to the wavelength of incident X-rays

Intensity of a diffracted X-ray beam as function of the grazing angle

The Dynamical Theory allows to calculate the amplitude of the wave field in a crystal and the intensity of the diffracted beam.

Here we consider only the (asymmetric) Bragg case:



We define:

$$\eta = [-b\,\Delta\theta_0 \sin 2\theta_B + (1/2)\,\Gamma F_0\,(1+b)] \,/\, \Gamma\,|P|\,|b|^{1/2}\,F_H$$

with

$b = [\sin(\theta - \alpha)] \,/\, [\sin(\theta + \alpha)]$ asymmetry parameter (b=1 for sym. Bragg case)

$\Delta\theta_0 = \theta_0 - \theta_B$

$\Gamma = (\lambda^2 / V\pi)\,(e^2/mc^2)$ with V = volume of unit cell

F_H Structure Factor for diffraction at lattice planes defined by the reciprocal lattice vector $\underline{H}$

$F_0 = (1 - \varepsilon) / \Gamma$ Structure Factor for $\underline{H} = \underline{0}$

P = 1 for σ polarisation
= cos 2 θ_B for π polarisation

η is generally a complex number: $\eta = \eta' + \eta''$, but gets real if absorption effects are neglected.

Now follows

$$|E_H|^2 \,/\, |E_0|^2 = |b|\,|\eta \pm (\eta^2 - 1)^{1/2}\,|^2$$

where

E_0 is the incoming electrical field
E_H is the diffracted electrical field
"-" is taken for $Re\{\eta\} > 0$ and "+" for $Re\{\eta\} < 0$

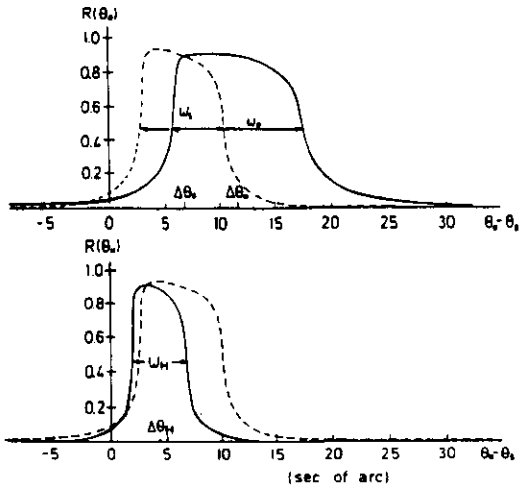


Fig. 4. Reflection curves for Si(111) at 1.6 Å. $R(\theta_0)$ is the reflectivity as a function of the incidence angle θ_0 while $R(\theta_H)$ represents the intensity reflected at a reflection angle θ_H for a plane wave incident at θ_0. (Solid lines for $b = 0.4$; broken lines for $b = 1$ where $R(\theta) = R(\theta_H)$.) From ref. [20].

We note that:

1. In a small angular range $\Delta\theta$ around θ_B the incident wave gets
   - quasi completely reflected
   - exponentially attenuated in the crystal

This attenuation is described by the Extinction Coefficient, which is much larger than the ordinary absorption coefficient (e.g. for Si, 20 keV: the extinction length is 20 μm, while the ordinary absorption length is 1.1 mm).

2. Outside of $\Delta\theta$ occurs no diffraction

3. the center of the diffraction curve is at $\eta'=0$
   and $\Delta\theta_0 = (1/2)\ (1 + 1/b)\ \Delta\theta_S$
   $\Delta\theta_H = (1/2)\ (1 + b)\ \Delta\theta_S$
   with $\Delta\theta_S = \Gamma\ F_0' / \sin 2\theta_B$

   This shift of the diffraction curve is due to the fact that the refraction index $n \neq 1$

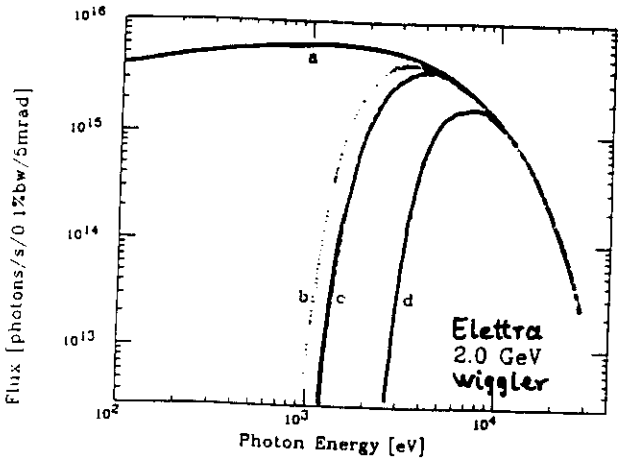
4. diffraction occurs in the range $-1 \leq \eta' \leq 1$
   with Darwin width $\omega_0 = \omega_S / b^{1/2}$
   $\omega_H = \omega_S\ b^{1/2}$
   where $\omega_S = 2\ \Gamma\ |P|\ F_H / \sin 2\theta_B$

Bragg reflection widths ω, energy resolutions $\Delta E/E$, and integral reflecting powers I of some reflections of Si, Ge and α-quartz perfect crystals at $\lambda = 1.54$ Å. From ref. [20].

Crystal	*hkl*	ω (second of arc)	$\Delta E/E$ ($\times 10^4$)	I ($\times 10^6$)
Silicon	111	7.395	14.1	39.9
	220	5.459	6.04	29.7
	311	3.192	2.90	16.5
	400	3.603	2.53	19.3
	331	2.336	1.44	11.8
	422	2.925	1.47	15.5
	333			
	(511)	1.989	0.88	9.9
	440	2.675	0.96	14.0
	531	1.907	0.60	9.3
Germanium	111	16.338	32.64	85.9
	220	12.449	14.46	67.4
	311	7.230	6.92	37.1
	400	7.951	5.94	42.3
	331	5.076	3.34	25.4
	422	6.178	3.34	32.4
	333			
	(511)	4.127	2.00	20.2
	440	5.339	2.14	27.5
	531	3.719	1.33	17.7
α-quartz	100	3.798	10.00	18.8
	101	7.453	15.26	40.9
	110	2.512	3.69	12.2
	$10\bar{2}$	2.488	3.36	12.9
	200	2.252	2.81	11.5
	112	2.927	3.03	15.5
	202	2.072	1.93	10.6
	212	2.042	1.47	10.7
	$20\bar{3}$	2.430	1.74	12.9
	301	2.368	1.69	12.6

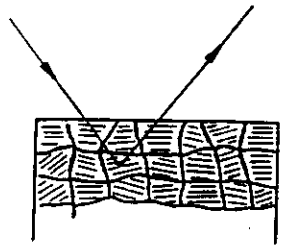
T. Matsushita & H. Hashizume, 1983

Solutions for heat load problem

① 

use power filters:

8 μm C
20 μm C
250 μm C

② 

Large band-pass optic:

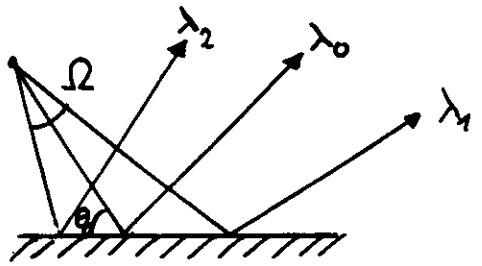
multilayers
mosaic crystals

③ cool 1. crystal very efficiently (3 kW absorbed!)
heat 2. crystal to match temperature:

diffraction beamline, Si(111) : $\Delta T \leq 13°C$
Si(220) : $\Delta T \leq 7°C$

3. Description of different monochromators

3.1 Single Crystal monochromator



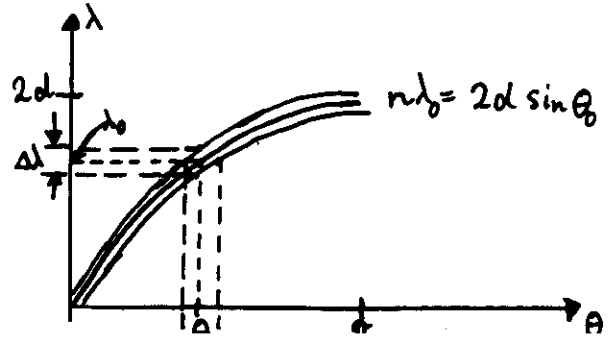
polychromatic point source with divergence Ω

$$\rightarrow \quad \lambda_0 = 2d \sin\theta_0$$
$$\lambda_1 = 2d \sin(\theta_0 - \Omega/2 - \omega/2)$$
$$\lambda_2 = 2d \sin(\theta_0 + \Omega/2 + \omega/2)$$

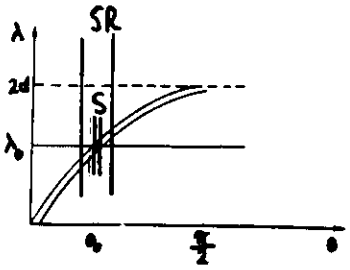
If Ω and ω small →

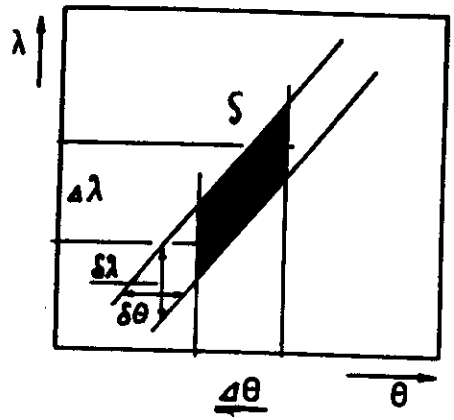
$$\Delta\lambda/\lambda = (\Omega+\omega)\cot\theta_0$$

= band pass



Du Mond diagram



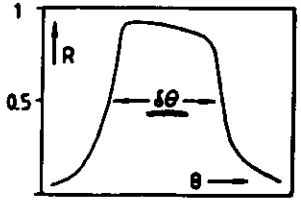


acceptance region composed by a crystal and a collimating slit S

- accepted photon flux ~ red area ↗

$\delta\theta$ = limited reflex width (Darwin width)
→ intrinsic spectral acceptance $\delta\lambda = \lambda \cot\theta \, \delta\theta$

$\Delta\theta$ = Divergence of incoming light beam
→ spectral resolution is given through red area ↗



as

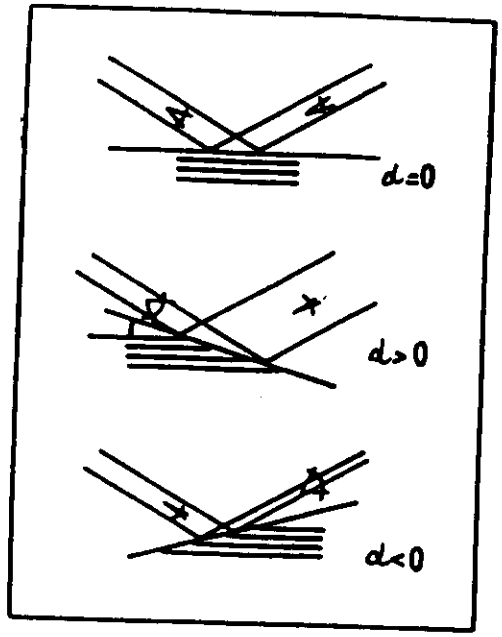
$$\frac{\Delta\lambda}{\lambda} = \cot\theta \, \Delta\theta + \frac{|\chi_h|}{\sin^2\theta}$$

with $|\chi_h| = \lambda^2 \frac{r_e}{\pi} \frac{|F_h|}{V_c}$

$r_e = 0.28 \cdot 10^{-12}$ cm
V_c = volume of unit cell

→ <u>accepted flux ~ $\delta\lambda \cdot \Delta\theta$</u>

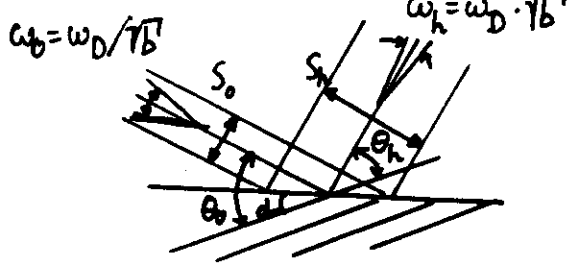
Asymetric Cut Crystals

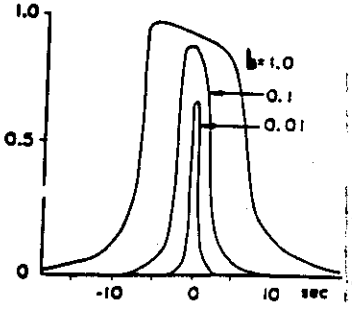


→ possibility to vary reflex width $\delta\theta$:

$$S_h \cdot \delta\theta_h = S_0 \cdot \delta\theta_0$$

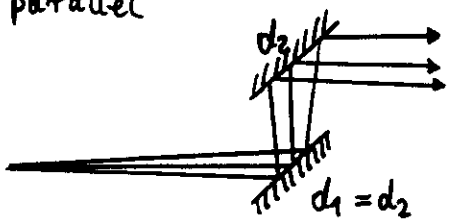
cross section S_0 of incoming beam
" S_h of diffracted "
$\Big\}: \frac{S_h}{S_0} = \frac{\sin(\theta-\alpha)}{\sin(\theta+\alpha)} =: b$



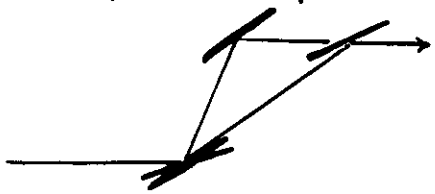


3.2 Two Crystal monochromators

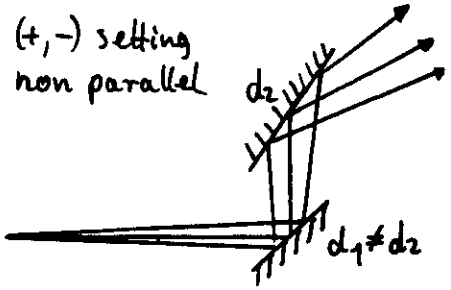
a) (+,−) setting parallel



- non dispersive
- fixed exit possible

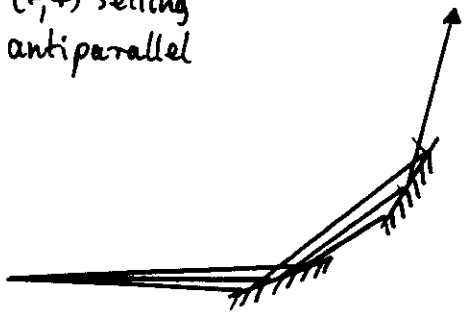


b) (+,−) setting non parallel



- dispersive (slightly)

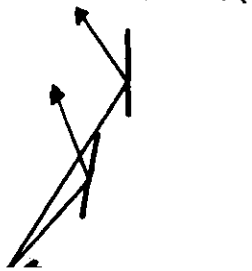
c) (+,+) setting antiparallel



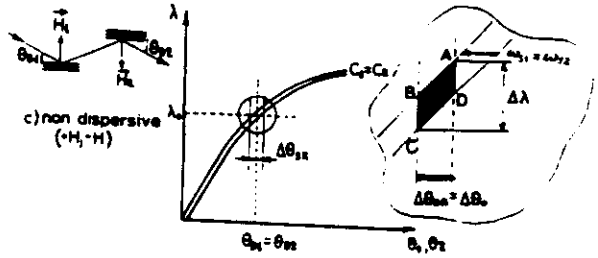
- highly dispersive

$\Delta\lambda/\lambda = \omega \cot\theta_0$

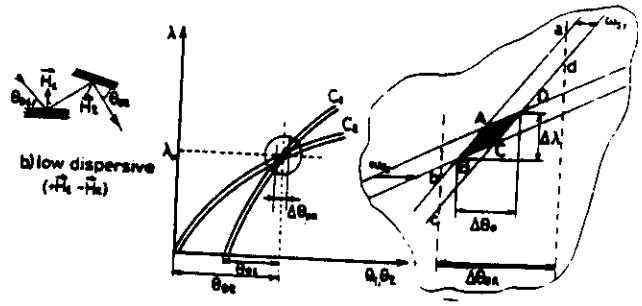
↑ intrinsic Darwin width

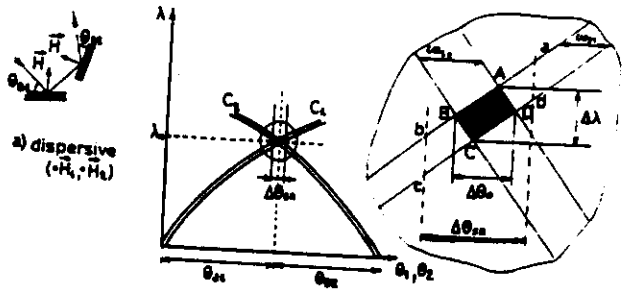


Du Mond diagrams



- highest intensity
- very good alignment required





- low intensity
- highly monochr.
- very stable configuration

Channel-Cut monochromator

One large monocrystal with a "channel"

→ • simplest two crystal monochromator
• naturally aligned
• cheap

but: • exit beam shifts vertically by

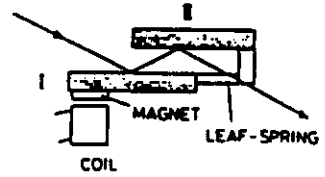
$$\Delta h = 2D \cos\theta_B$$, with D = distance between crystal surfaces

• higher order problem

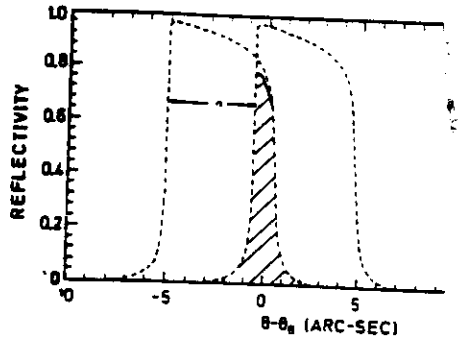
resolution: $\frac{\Delta\lambda}{\lambda} = (\Omega_{\substack{Real\\Source}} + \Omega_{slit} + \omega_h/\sqrt{b}) \cdot \cot\theta_B$

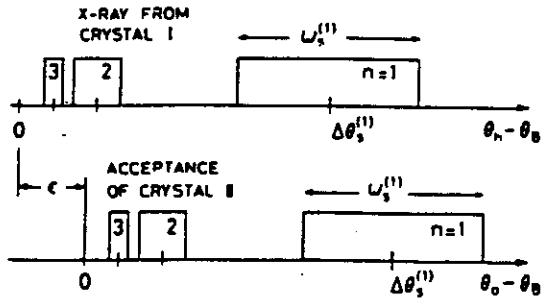
with $\Omega_{\substack{Real\\Source}}$ = vertical divergence on crystal given by the vertical source size = S/L

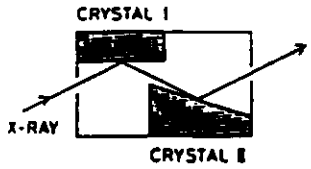
Ω_{slit} = vertical divergence on crystal given by the entrance slit = F/L

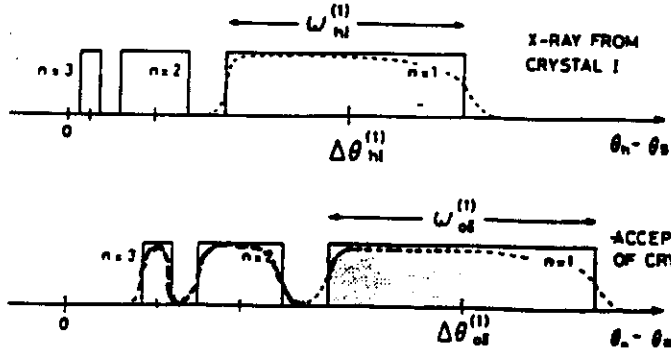


(a)

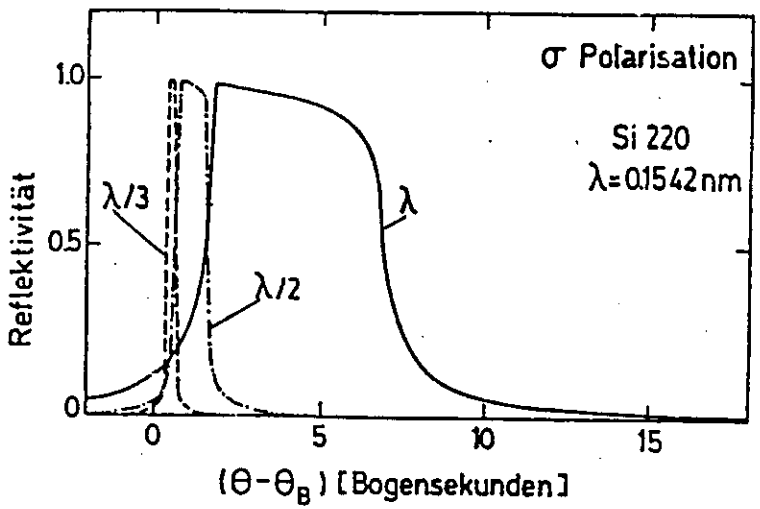






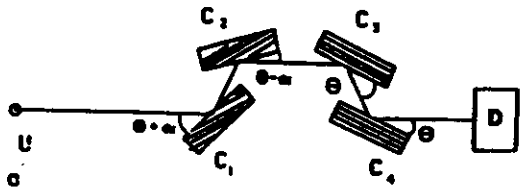


Materlik + Graeff 1982



4 crystal monochromator

- highly dispersive + fixed exit



4 crystal dispersive

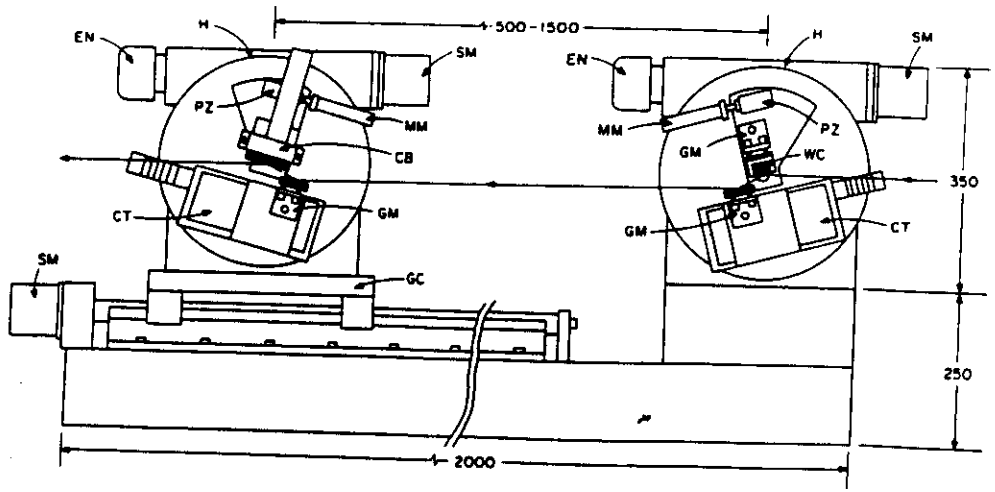


Fig. 3. Schematic of the monochromator. CB: crystal bender; CT: crystal translation stage; EN: encoder; GC: goniometer carriage for 1 m translation; GM: gimbal mount for prealigning crystal; H: Huber model 421 goniometer; MM: motorized micrometer for coarse alignment; PZ: piezoelectric translator for fine crystal alignment; SM: stepping motor; WC: water cooled crystal. Not shown is the piezoelectric adjuster for adjusting the angle of the first goniometer.

S. Heald et. al., NIM 222, 160 (1984)

Focussing X-rays

mirror

- 1 optical element for sagittal + tangential focussing possible
- cut-off frequency → very grazing incidence → very long mirrors (typ. > 1 m !)
- high requirements for
  - slope errors (< 2 arc sec)
  - surface roughness (< 5 Å)
  - alignment
- expensive

crystal

- 2 crystals needed
- since radius of curvature $R_{crystal} \gg R_{mirror}$ → ~ 10× acceptance (geometrical)
- small crystals → cheaper

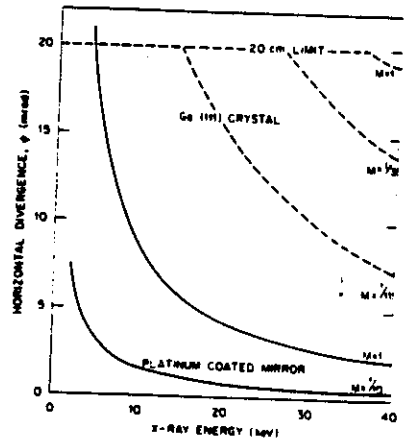
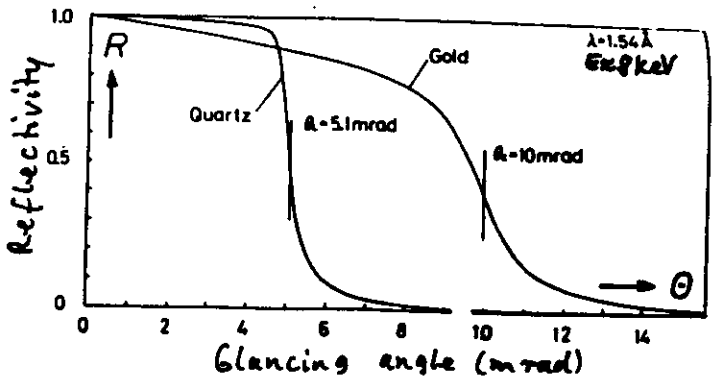


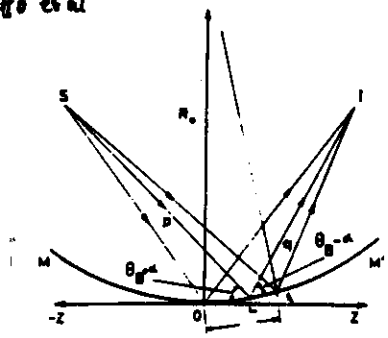
Fig. 1. Comparison of the horizontal divergence intercepted with sagittal focusing by a Ge(111) crystal and platinum-coated mirror located 10 m from the radiation source as a function of photon energy and magnification, M. The crystal dimension is limited to 20 cm with no size restriction placed on the mirror.

C.J. Sparks et al
NIM 172, 237 (1980)

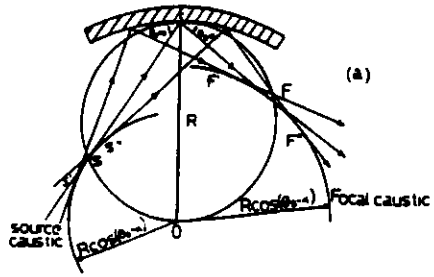
$\sin\theta_c = \lambda\sqrt{\frac{e^2 N}{mc^2\pi}}$, N = No. e^- per unit volume



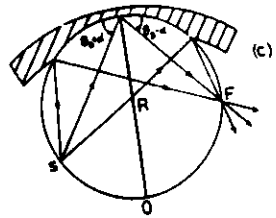
R. Caciuffo et al
1987



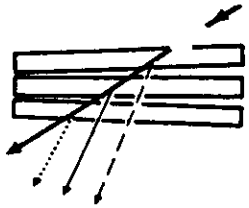
$$\frac{2}{R} = \frac{\sin(\theta_B + \alpha)}{p} + \frac{\sin(\theta_B - \alpha)}{q}$$



Johann



Johansson



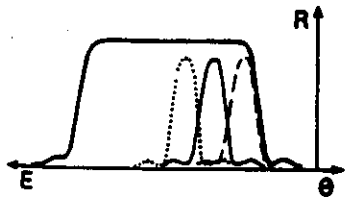
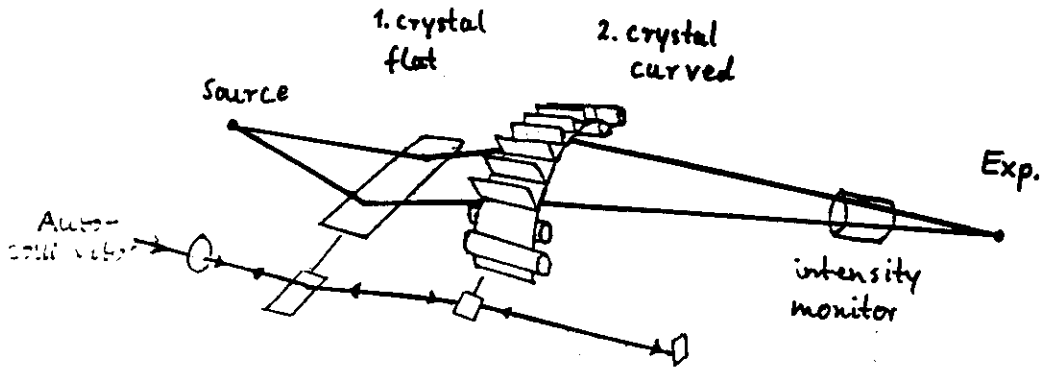


FIG. 3. Calculating of the reflectivity curve from the lamellar model. Reflection of a parallel polychromatic beam is shown above, and below the reflectivity curves of individual lamellas with their sum, the reflectivity curve of the bent crystal R, as a function of energy E, or angle θ.

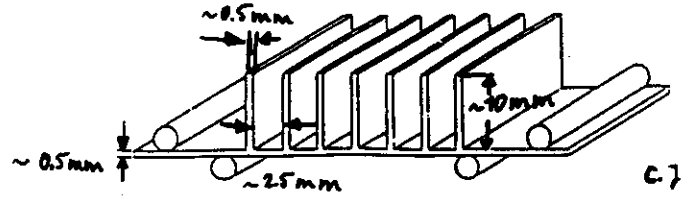
P. Suortti, Rev. Sci. Instrum., Vol. 63, No. 1, ... ary 1992
p. 942



Two feedback-systems: 1. keeps crystals // to 1arcsec

2. ionisation chamber →

detuned mode for higher order suppression

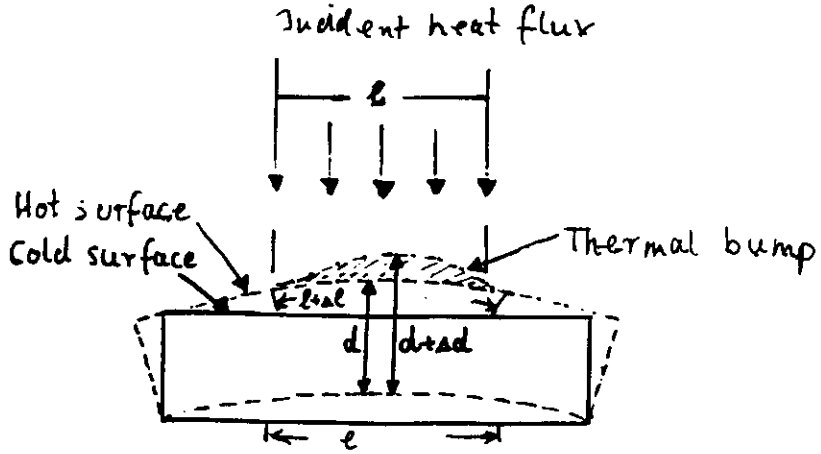


C.J. Sparks et al.
Nucl. Instr. & Meth.
194, 73 (1982)

4-bar bending device → cylindrical and conical shapes

R = 1.5 ↔ 40 m

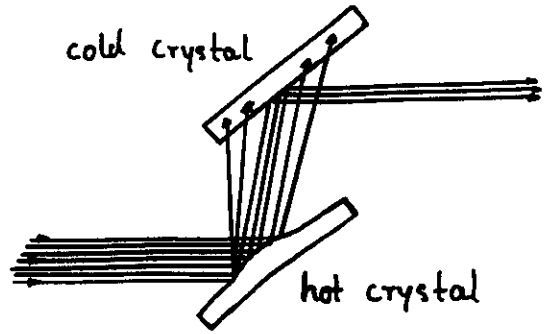
Heating effects



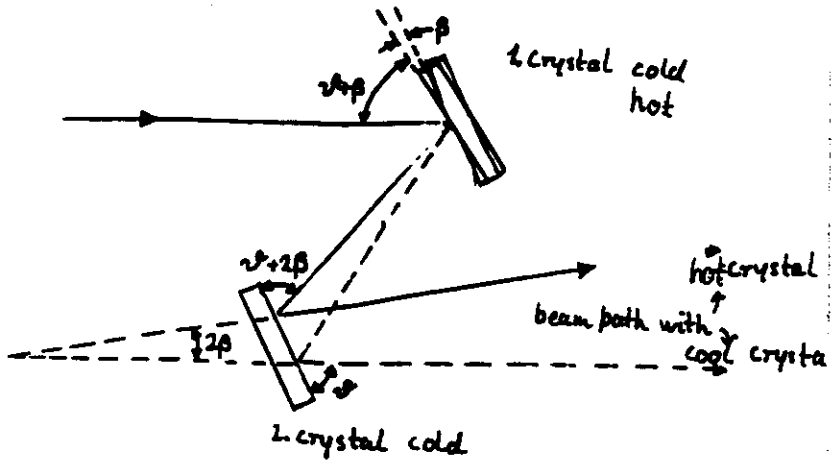
Deformations of a monochromator crystal:

1. overall bending
2. "thermal bump"

① loss of throughput intensity

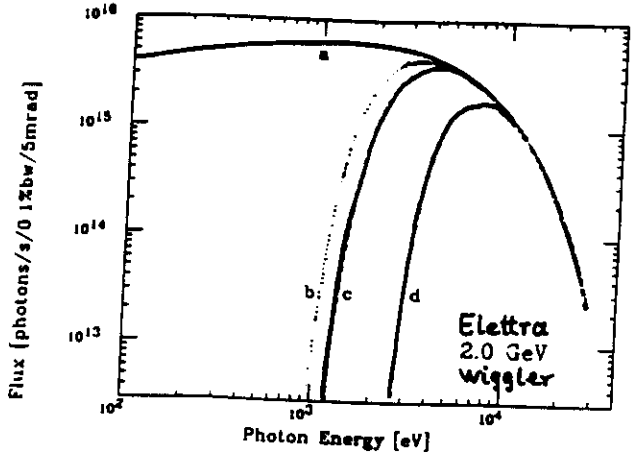


② Loss of intensity requires detuning → shift of exit beam



Solutions for heat load problem

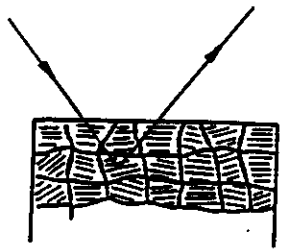
①



use po
filters

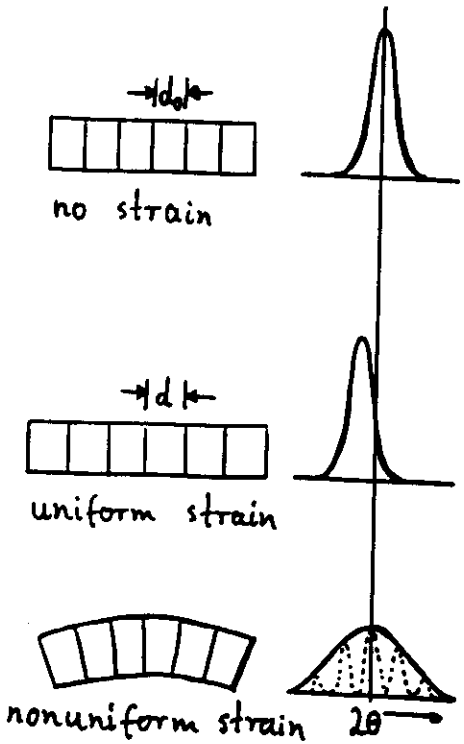
8 μm
20 μm
250 μm

②



Large band-pass op

multilayers
mosaic crystals



③ loss of energy calibrati

③ cool 1. crystal very efficiently (3 kW absorb
heat 2. crystal to match temperature:

diffraction beamline, Si(111) : $\Delta T \leq 13°C$
Si(220) : $\Delta T \leq 7°C$

④ line broadening

$$b = 2\frac{\Delta d}{d}\tan\theta$$

Advanced cooling schemes internal cooling with H_2O

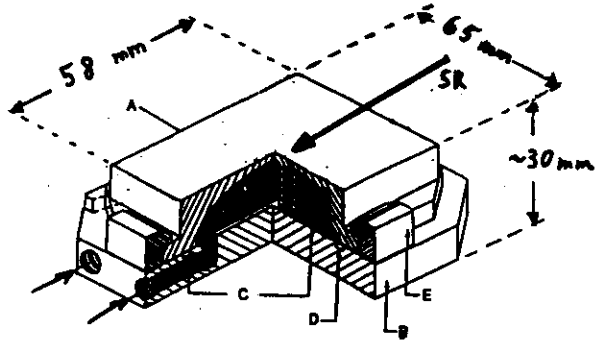
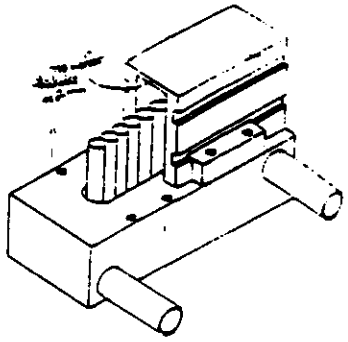
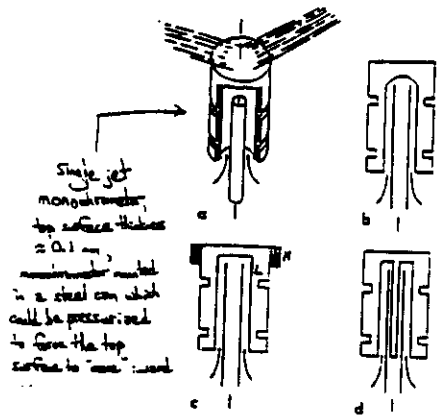


Fig. 2a: Schematic drawing of a cooling scheme. A: Si-crystal; B: copper cooling substrate; C: passages for cooling fluid; D: O-ring seal groove; E: crystal clamp block

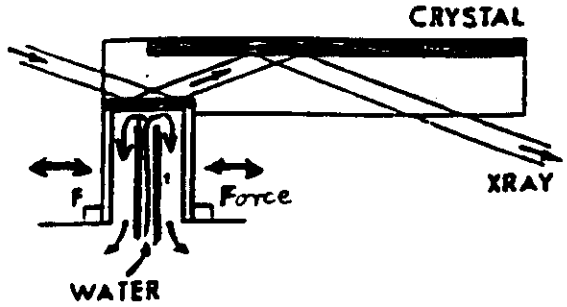
(T. Oversluizen et al, Rev. Sci. Instr. 60, 1493 (1989))

Advanced Cooling Methods





Hart 1990 : Figure 4.



waterjet + dynamic bending

(Hart, Uni Manchester)

Crystal materials

Requirements:

- energy range + resolution (given by experiment)
- no absorption edges
- heat and radiation resistance
- high reflectivity
- available in sufficient sizes
- "easy" to manufacture
- low cost
- small mosaic spread

Energy resolutions of the monochromator required in various experiments.

Experiments	$\Delta E/E$ or $\Delta\lambda/\lambda$
X-ray microscopy	$10^{-1} - 10^{-2}$
Structure analysis	$10^{-1} - 10^{-3}$
Compton scattering	$10^{-2} - 10^{-4}$
EXAFS	$10^{-3} - 10^{-4}$
Topography (white beam)	$(10^{-3} - 10^{-4})^{*}$
Anomalous scattering	$\sim 10^{-4}$
Interferometry	$\sim 10^{-4}$

Table 5
Soft X-ray monochromator crystals.

Crystal	2d	Energy region/eV	Comments
Si (111)	6.2706	2000–[illegible]	Good stability
Ge (111)	6.532	2000–[illegible]	
In Sb (111)	7.4806	1690–4000	
α-Quartz (10$\bar{1}$0)	8.512	1480–3700	
Beryl (10$\bar{1}$0) ($Be_3Al_2(SiO_3)_6$)	15.92	800–2000	0.6 eV resolution at 1000 eV
Mica (002)	19.84	840–1600	
Sodium β-alumina ($Na_2O \cdot 11Al_2O_3$)	22.49	550–1500	
KAP (Potassium acid phthalate)	26.6 Å	470–1300	Resolution ~1 eV radiation damage
Synthetic layered structures, e.g., C-W, B-W, Nb-C	from 10 Å upwards		Enormous possibilities

Si (220)
YB_{66}

6–30 keV

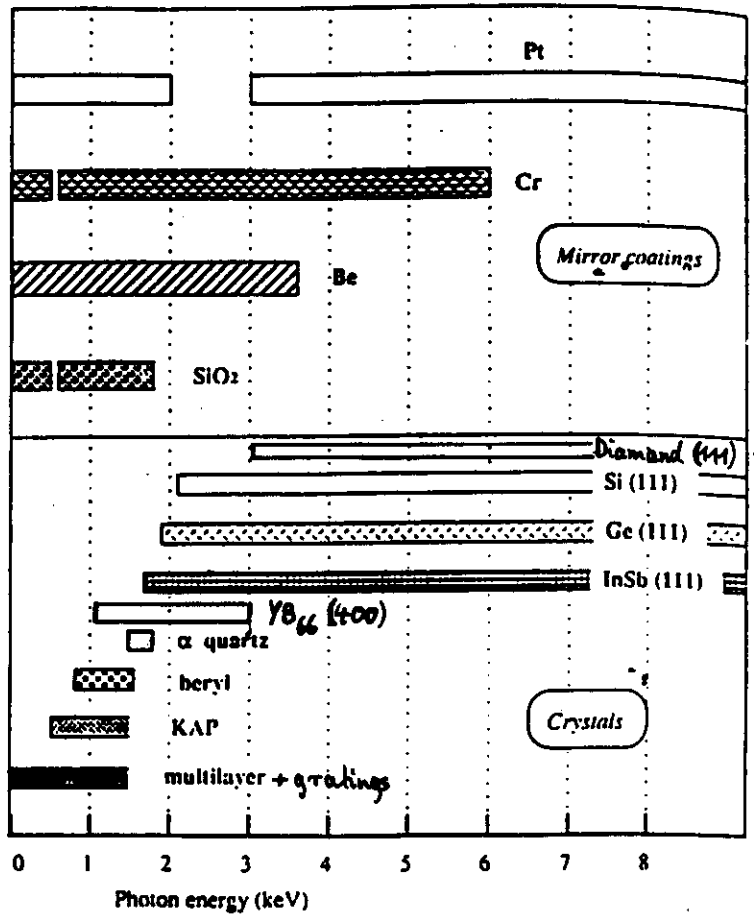


Fig. 3. Energy regions for reflecting coatings ($\alpha = 0.45°$) and monochromator crystals ($10 < \theta < 80°$)

Monochromators

- 5 – 30 eV : normal incidence, grating
- 10 – 1000 eV : grazing incidence, grating
- > 800 eV : crystals

Absorption edges in crystals

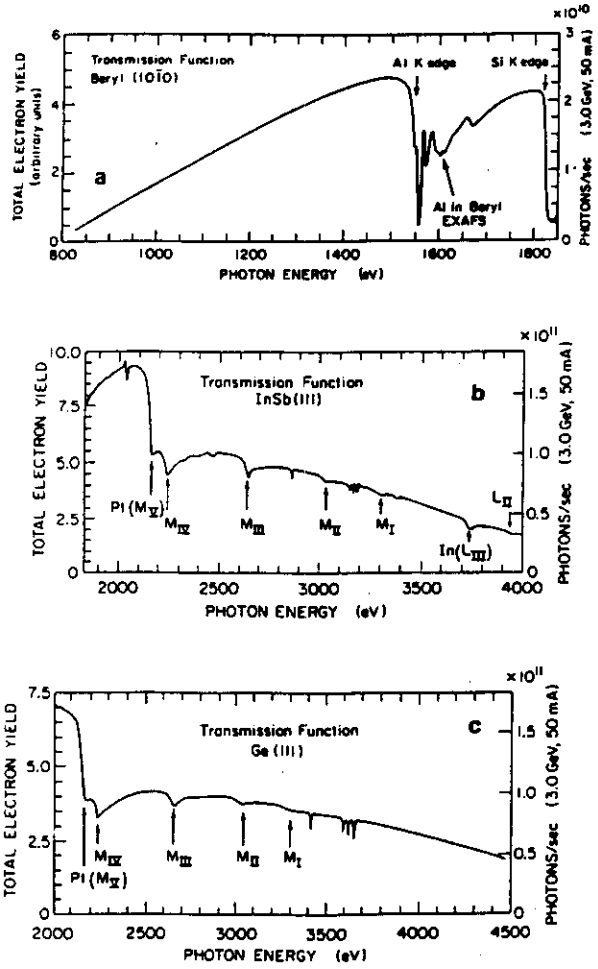


Fig. 39. Transmission functions for the SSRL double crystal monochromator: (a) Beryl (10$\bar{1}$0), (b) InSb (111), (c) Ge (111) (courtesy Lawrence Berkeley Laboratory, University of California).

Literature

First publications on crystal therories:

1. C. G. Darwin, Phil. Mag.**27**, 315, 675 (1914)
2. P. P. Ewald, Ann. Physik **49**, 1,117 (1916); **54**, 519 (1917)
3. M. von Laue, Ergeb. Exakt. Naturw., **10**, 133 (1931)

Introductions into the different forms of Dynamical Theory:

4. R. W. James, Optical Principles of the Diffraction of X-Rays, G. Bell and Sons, London, 1950
   R. W. James, Solid State Physics, Vol 15, Academic Press, New York, 1963
5. W. H. Zachariasen, Theory of X-Ray Diffraction in Crystals, John Wiley and Sons, Inc., New York, 1945 (New edfition by Dover, New York, 1967)

Important extensions to and summaries of the Dynamical Theory are contained in e.g. the following articles:

6. P. B. Hirsch, Acta Cryst. **5**, 176 (1952), and P. B. Hirsch and G. N. Ramachandran, Acta Cryst. **3**, 187 (1950)
7. N. Kato, J. Phys. Soc. Japan 7, 397 (1952)
8. G. Borrmann, Trends in Atomic Physics, Interscience Publishers, Inc., New York, 1959
9. K. Kohra, X-Ray Crystallography (Maruzen Co. Ltd, Japan 1961), Vol.II, 9, P. 849
10. A. Authier, Bull. Soc. Franc. Mineral. Crist., **84**, 51 (1961)

A complete summary of the Ewald - von Laue formulation of the Dynamical Theory is given in the review article by

11. B. W. Batterman and H. Cole, Rev. Mod. Phys. **36**, 681 (1964)

Further Review Articles on Crystal Theories and X-Ray Optics:

- Jackson, Classical Electrodynamics, Wiley
- R. W. James, The Optical Principles of the Diffraction of X-Rays, Bell, London, (1965)
- B. E. Warren, X-Ray Diffraction, Addison-Wesley Publishing Company, Reading, M.A., (1969)
- T. Matsushita & H. Hashizume, Handbook on Synchrotron Radiation, Vol. 1A, Ch. 4, ed. E.E. Koch, North Holland, (1983)
- R. Caciuffo, S. Melone, F. Rustichelli and A. Boeuf, Physics Reports **152**, 1, (1987)

Recommended Journals for X-ray Optics:

- Nucl. Instr. & Methods (with special sections on use of Synchrotron Radiation)
- Review of Scientific Instruments (with special sections on use of Synchrotron Radiation)
- Journal of Applied Crystallography