AP6180/AP8180
Modern Scattering Methods in Materials Science

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Fundamentals of X-ray scattering

香港城市大學
City University
of Hong Kong

Fundamentals of X-ray scattering

Brief history
Laboratory X-ray sources,
Basic properties of X-rays,
X-ray spectra,
X-ray absorption edges,
Synchrotron X-ray sources,
Scattering mechanisms of X-rays by matter,
Atomic scattering factors for X-rays
Total X-ray reflection,
Darwin-breadth (qualitatively)
Monochromators (briefly)

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Brief history

Reading:

B.E.Warren, X-ray Diffraction,
Dover Publ., 1969, 1990

B.D.Cullity & S.R.Stock, Elements of X-ray Diffraction
Prentice Hall Inc. 2001

P.Klug & L.E.Alexander, X-ray diffraction procedures
for polycrystalline and amorphous materials,
Wiley, NY, 1954

L.H.Schwartz & J.B.Cohen, Diffraction from Materials,
AP. Academic Press, 1977

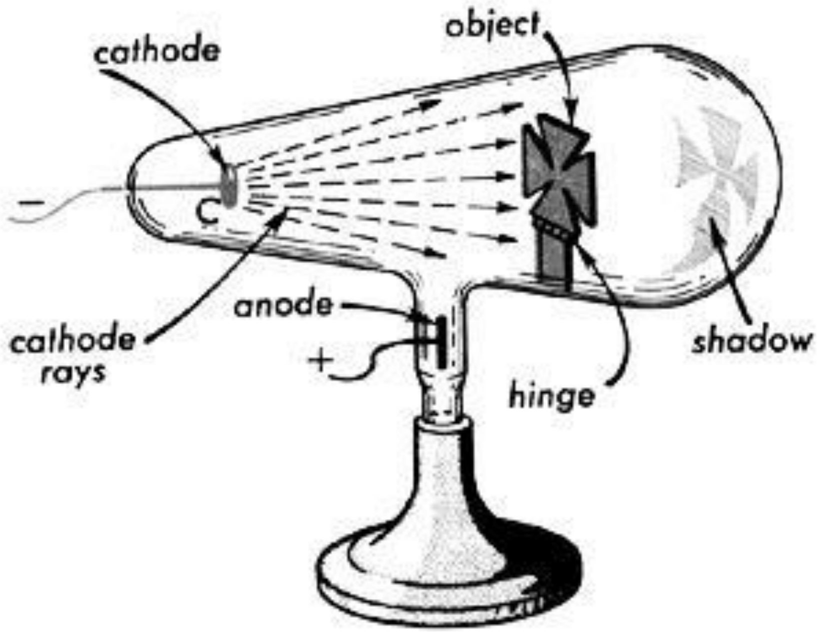
The tale:

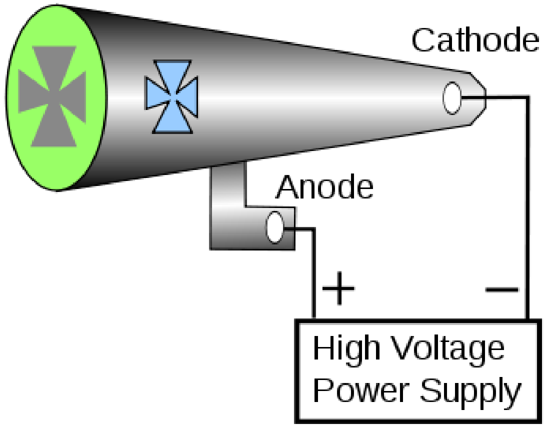
Röntgen, a German physicist,
was experimenting with a Crookes tube
when it produced streams of electrons
called cathode rays.
Just before leaving for lunch one day,
Röntgen put an activated tube on a book and
the book just happened to be lying on
a piece of photographic film.
Inside the book was a key and
when he later discovered that image,
he knew he was looking at
something entriely new.
The world's first ever x-ray

Wilhelm Konrad Röntgen
1845 - 1923

Discovery: 1895, Nobel Prize: 1901

William Crookes
(1832-1919)

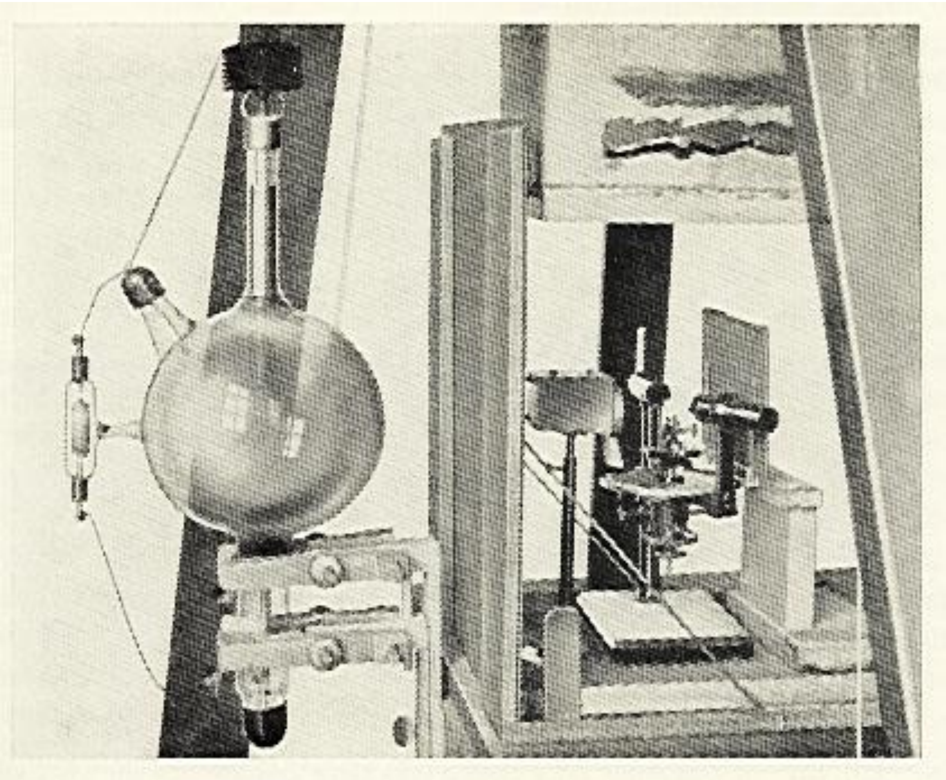


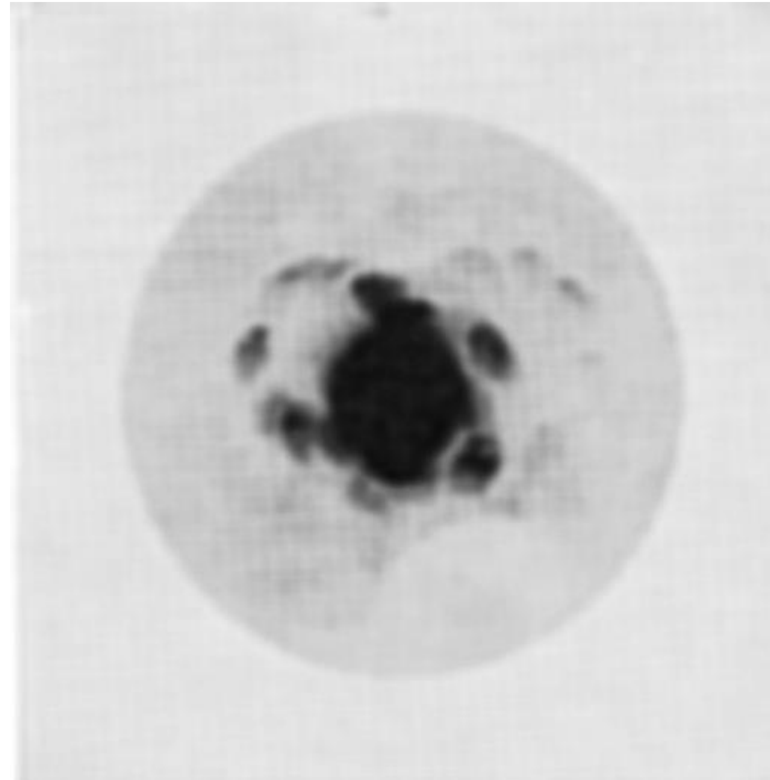


Crookes tube

X-ray or röntgen image of one of the hands of Röntgen's wife

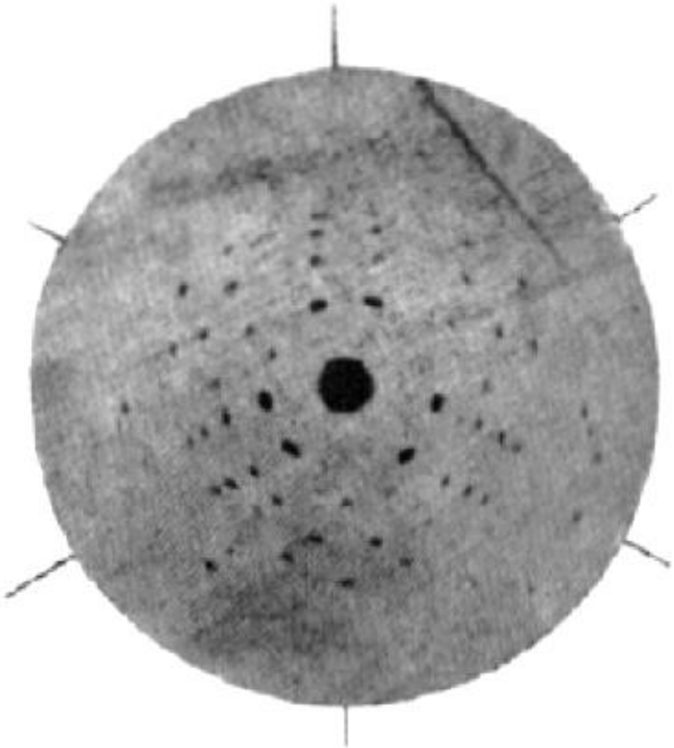
the first diffraction experiments: Max von Laue, 1912

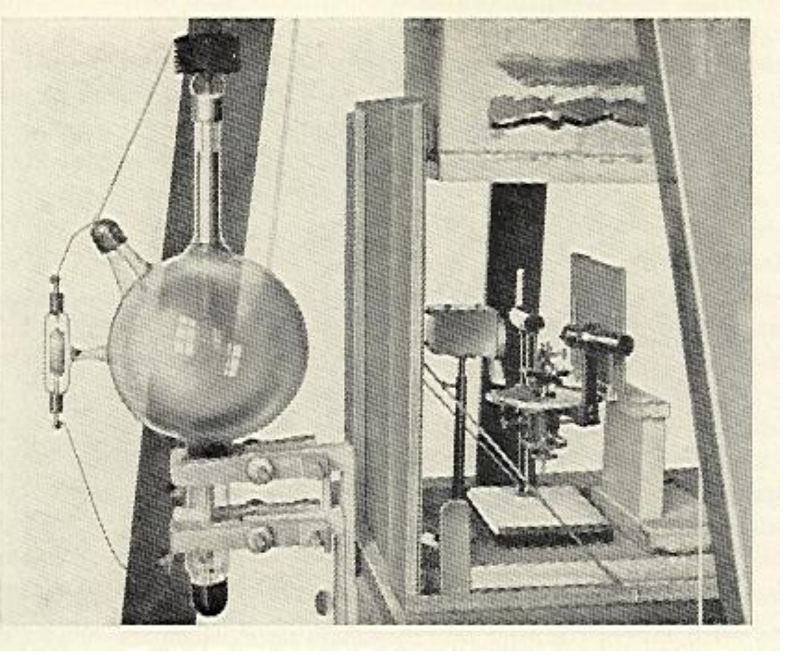




Laue photograph of zinc blend, ZnS
along the three-fold axis
M.vonLaue, Friedrich & Knipping, 1912

the first diffraction experiments: Max von Laue, 1912





third improved image,
after applying a pinhole

Laue photograph of zinc-blend, ZnS
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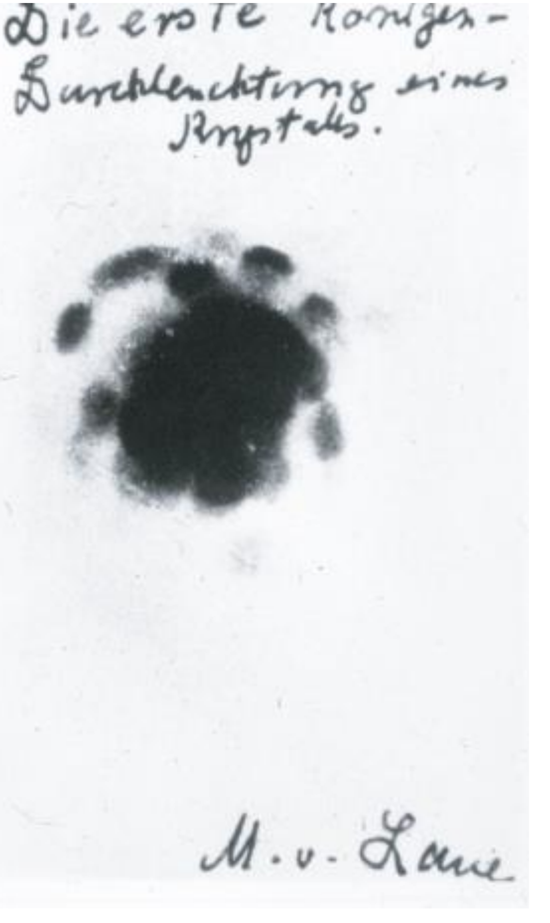
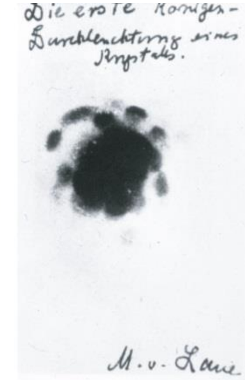


the first diffraction experiments: Max von Laue, 1912



two consequences

1) materials are crystalline consisting of atoms
2) X-rays are waves

electromagnetic waves

Nobel Prize in Physics 1914

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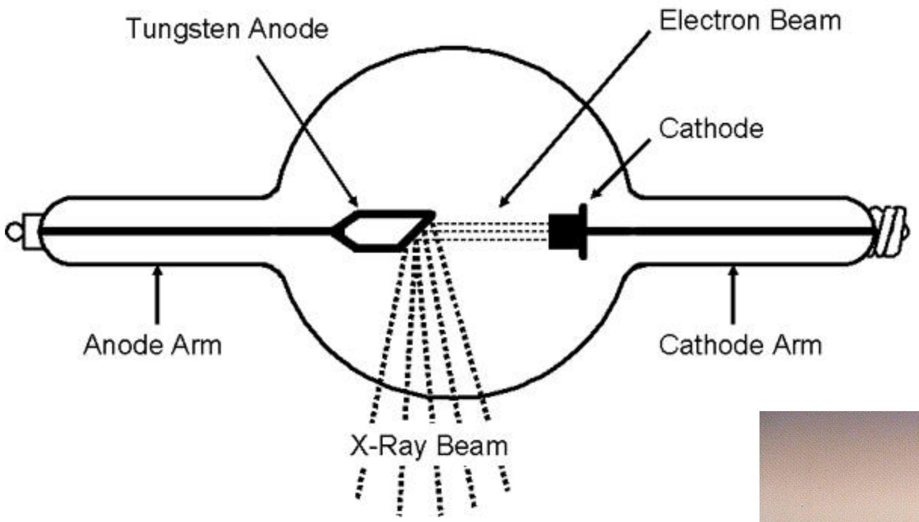
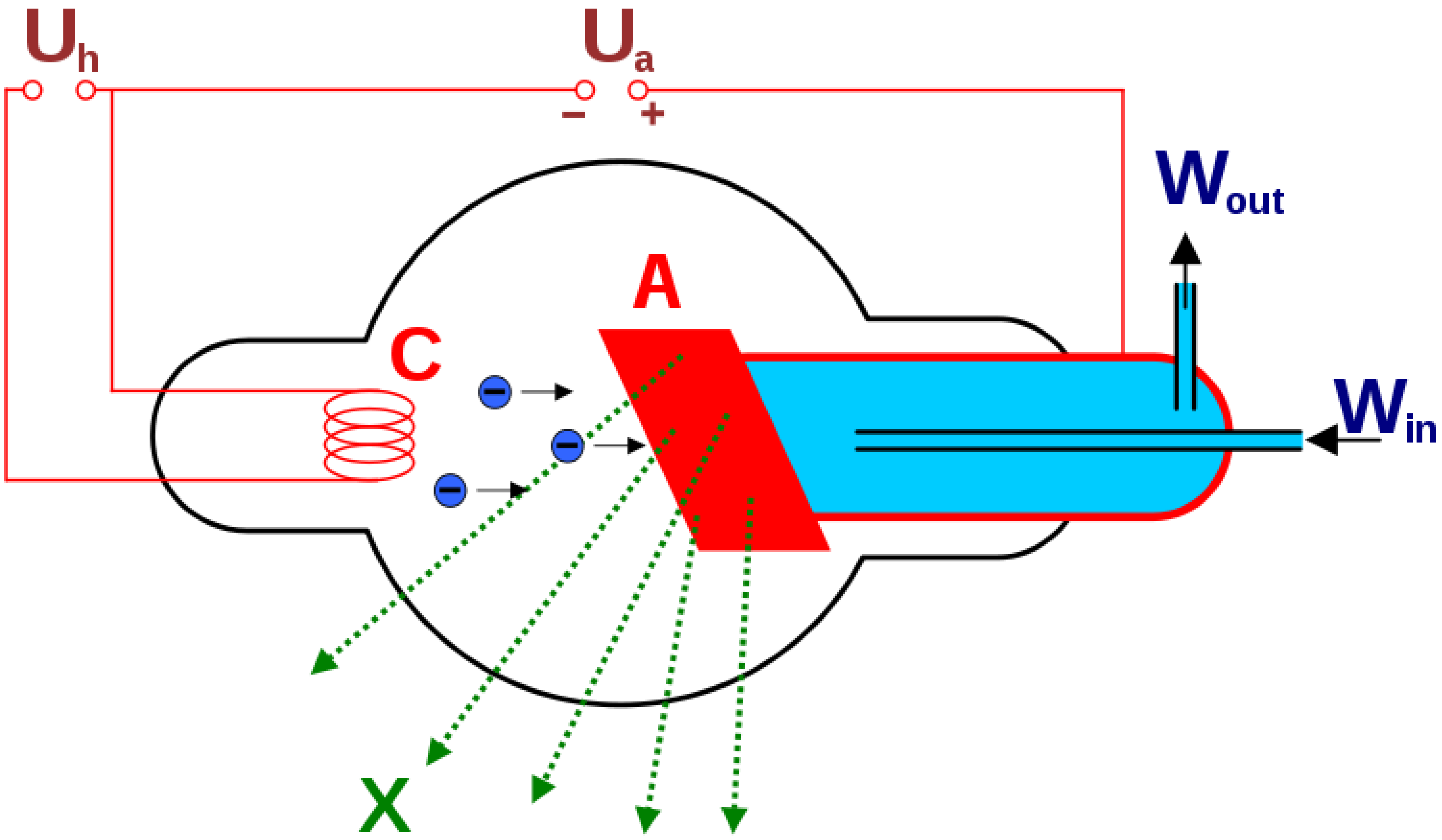
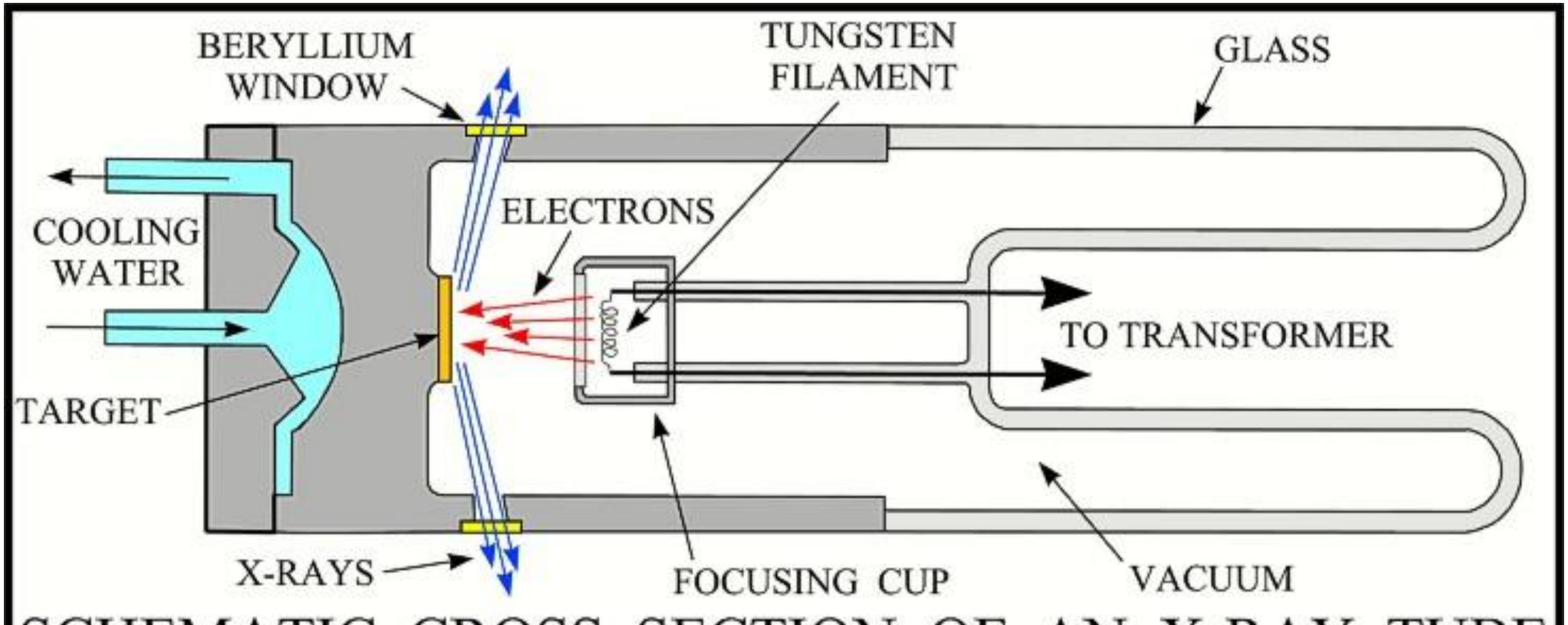
the first X-ray tubes:



the first X-ray tubes:



X-ray tubes today



SCHEMATIC CROSS SECTION OF AN X-RAY TUBE

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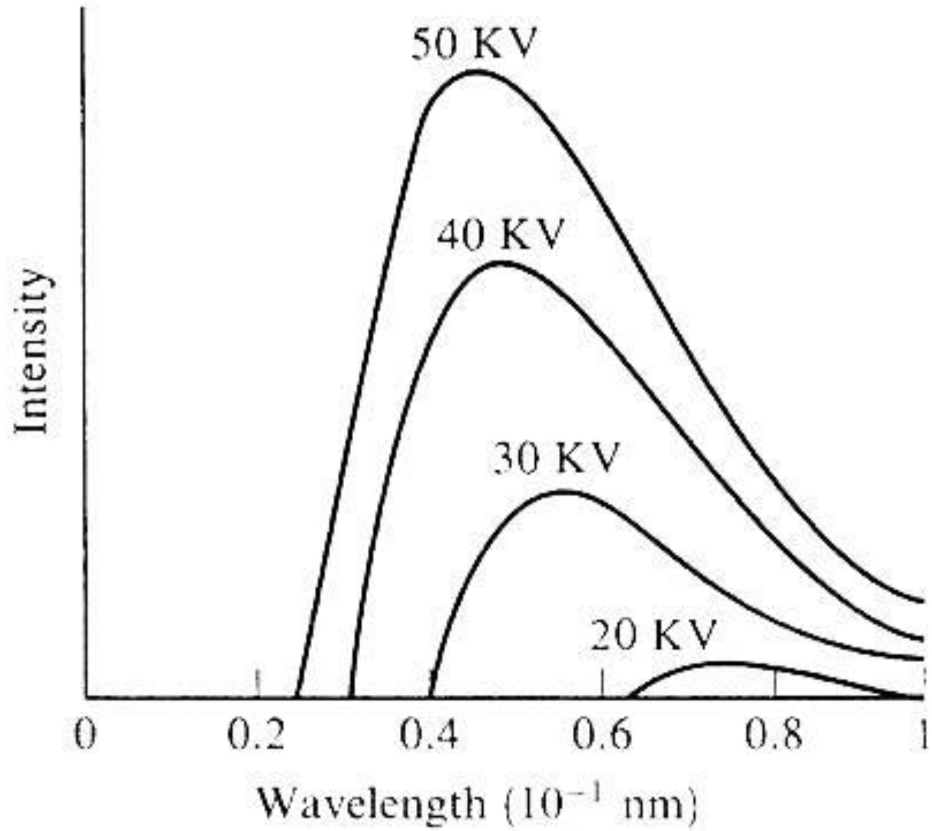
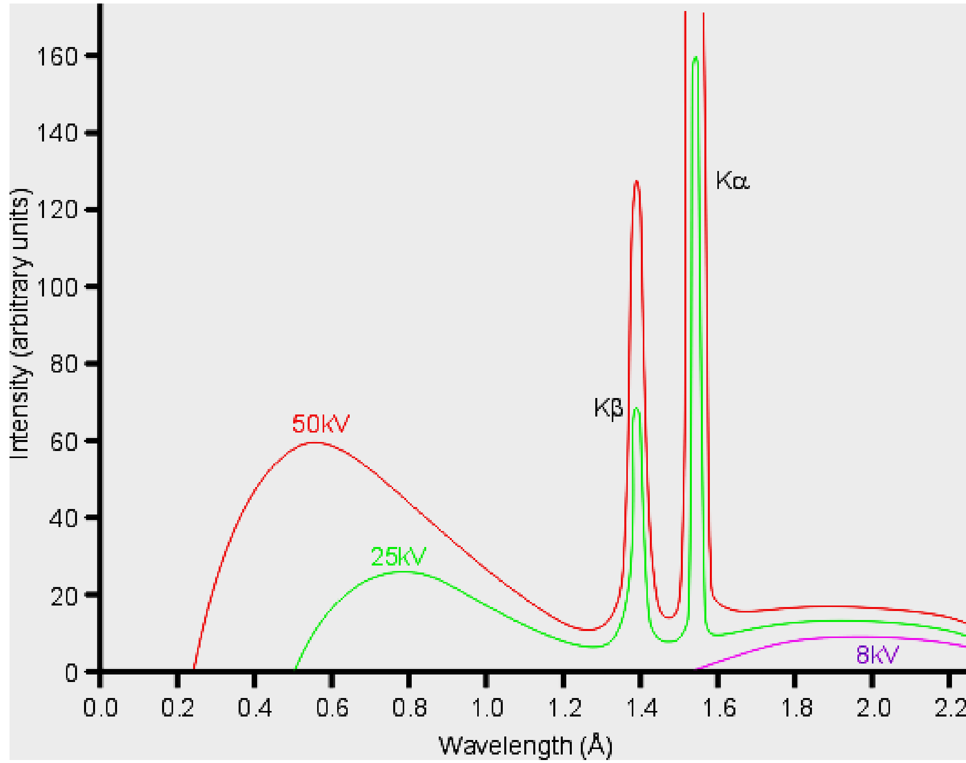
X-ray spectra



bremsstrahlung

radiation produced by random inelastic scattering by the electrons in the material

X-ray spectra



characteristic X-ray spectrum

radiation produced by
when the exited atom relaxes
by emitting a photon

X-ray spectra

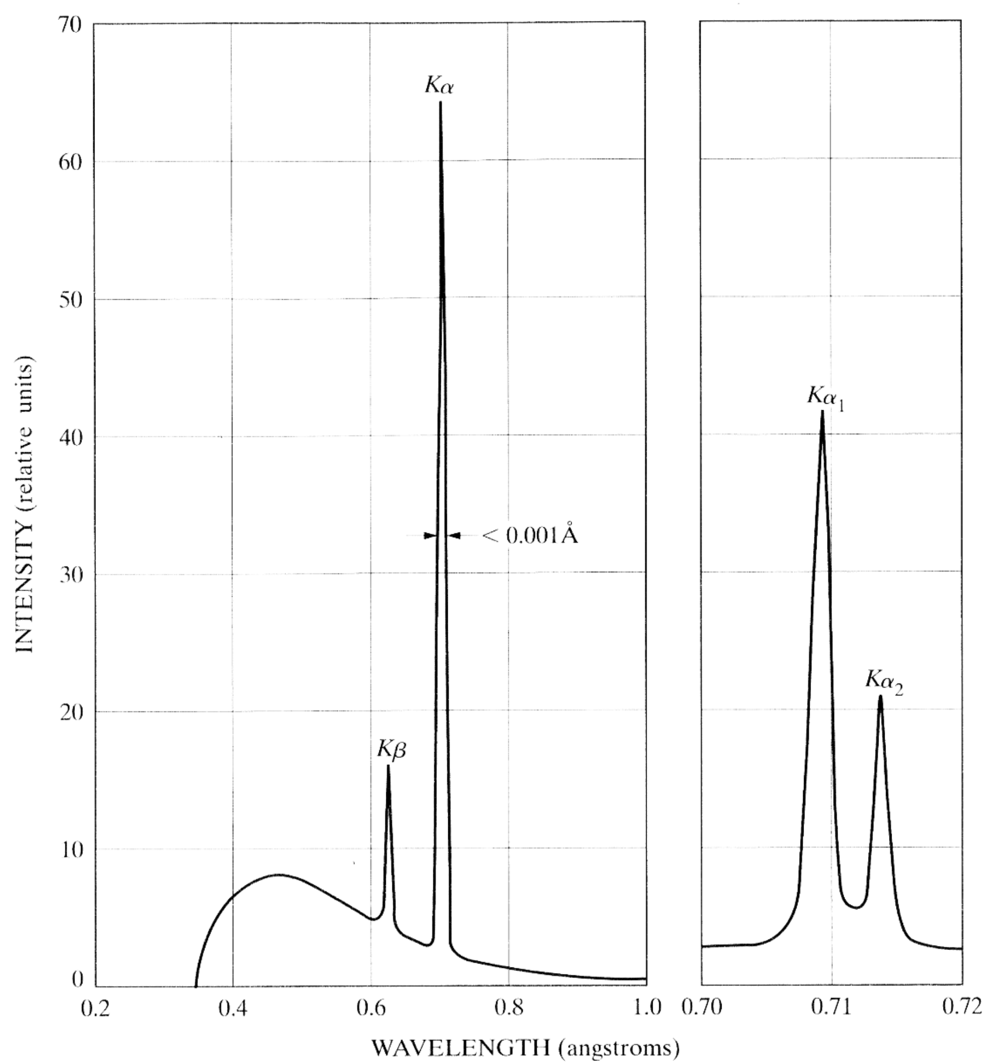


Figure 1-5 Spectrum of Mo at 35 kV (schematic). Line widths not to scale. Resolved $K\alpha$ doublet is shown on an expanded wavelength scale at right.

characteristic X-ray spectrum

radiation produced by
when the exited atom relaxes
by emitting a photon

X-ray spectra

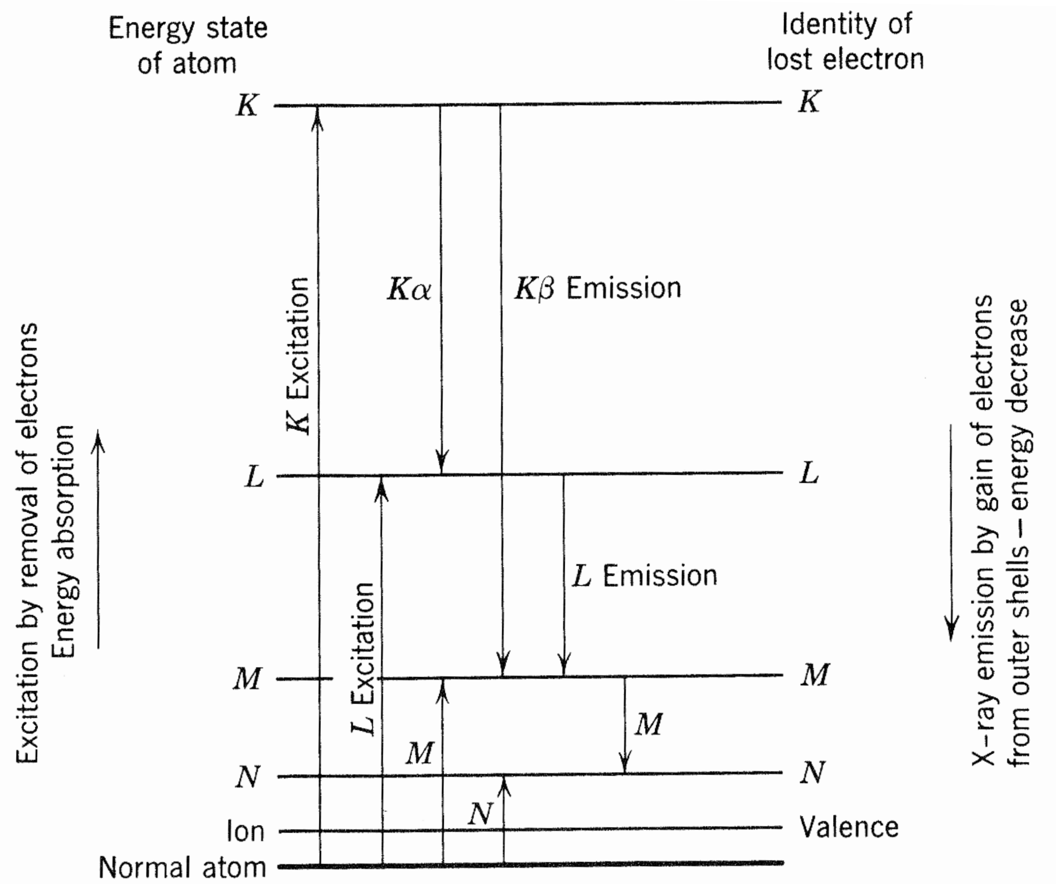


Fig. 2-16. Schematic energy-level diagram for a many-electron atom, indicating (by arrows) the processes of excitation and emission.

X-ray spectra

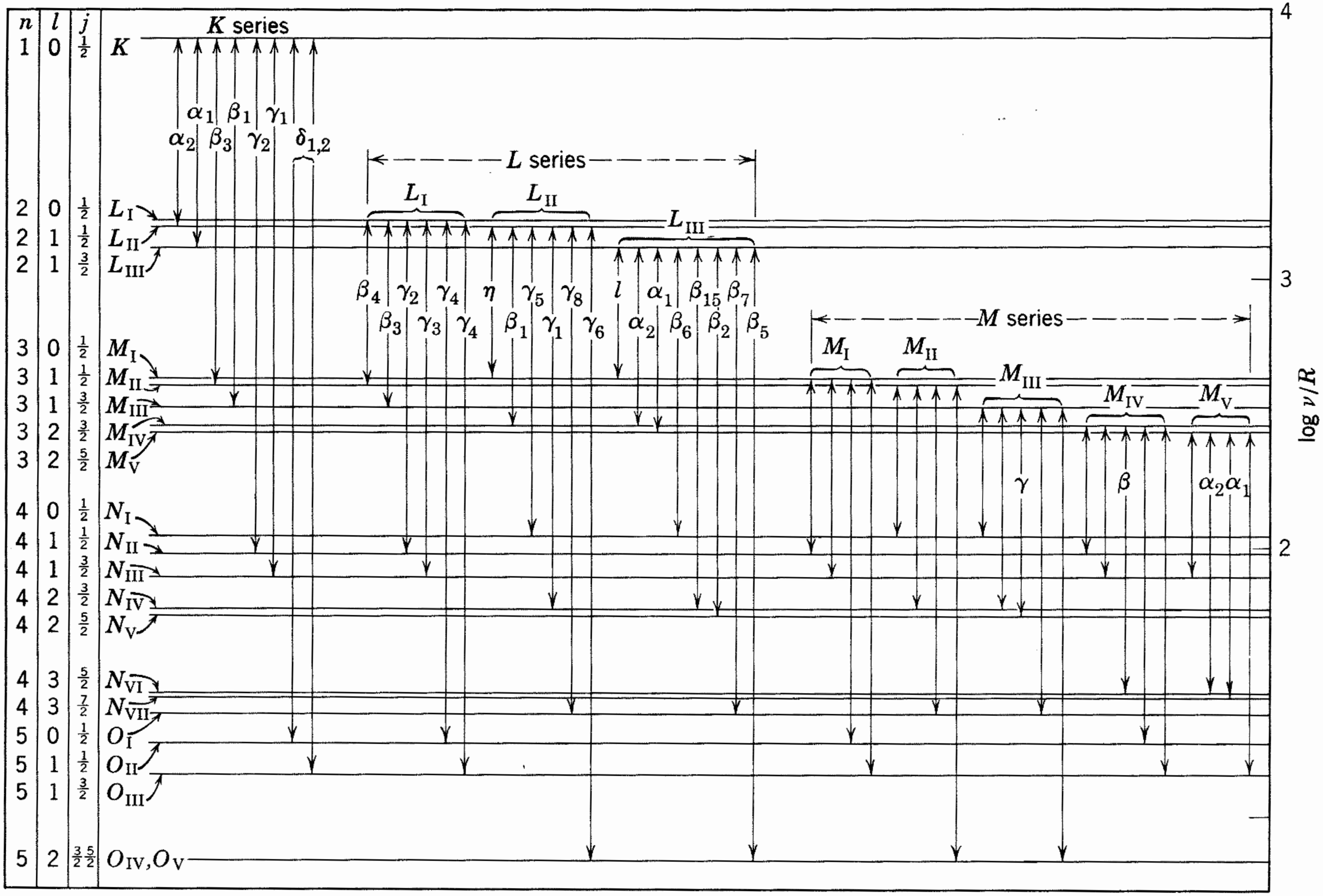


Fig. 2-17. X-ray energy-level diagram for uranium 92. (By permission, from F. Richtmyer and E. Kennard, *Introduction to Modern Physics*, Copyright, 1947, McGraw-Hill.)

X-ray wavelengths used in the laboratory

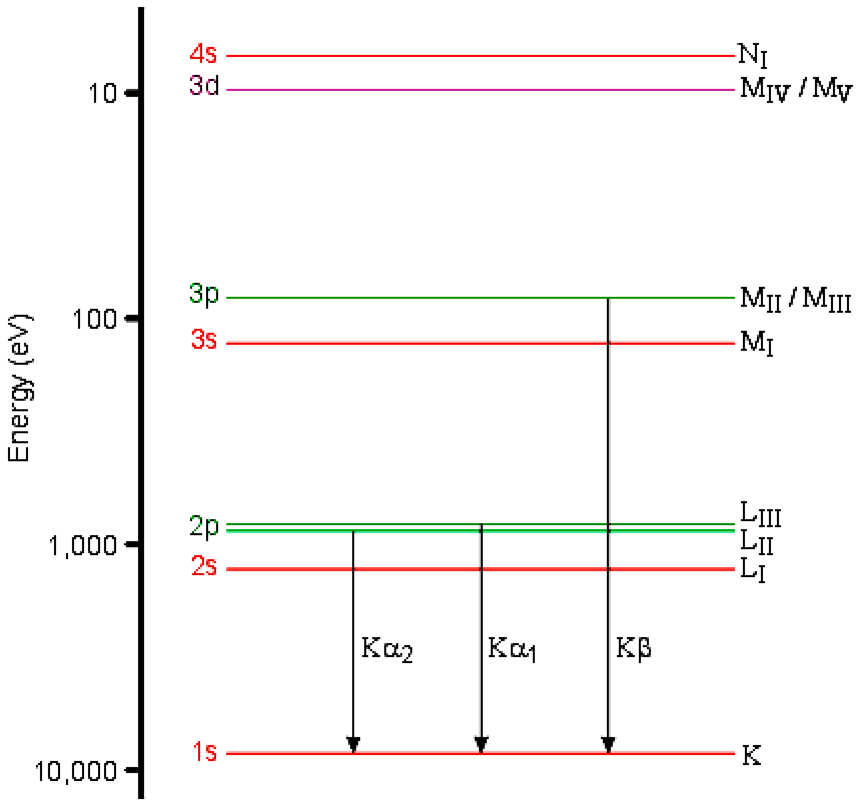
Table 2-3. X-ray Wavelengths Most Useful in Diffraction Studies[a]

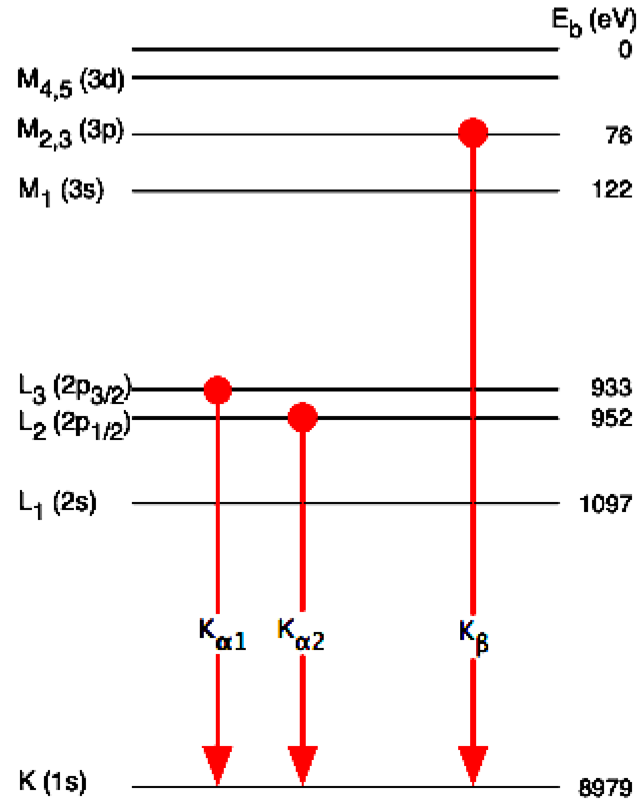
Element	$K\alpha_1$ (Å)	$K\alpha_2$ (Å)	Unresolved[b] $K\alpha$ (Å)	$K\beta_1$ (Å)	K Absorption Edge (Å)	Excitation Potential (kV)
Ag	0.55941	0.56380	0.56084	0.49707	0.4859	25.52
Mo	0.70930	0.71359	0.71073	0.63229	0.6198	20.00
Cu	1.54056	1.54439	1.54184	1.39222	1.3806	8.98
Ni	1.65791	1.66175	1.65919	1.50014	1.4881	8.33
Co	1.78897	1.79285	1.79026	1.62079	1.6082	7.71
Fe	1.93604	1.93998	1.93735	1.75661	1.7435	7.11
Cr	2.28970	2.29361	2.29100	2.08487	2.0702	5.99

[a] These values are taken from Bearden [43] in which they were listed on a re-adjusted scale of Å* units based on $\lambda(WK\alpha_1) = 0.2090100$ Å*. Since 1 Å* = 1 Å to ±5 ppm (probable error), values in this table are designated as being in ångström units.

[b] These values are the customary weighted mean of $K\alpha_1$ and $K\alpha_2$, $K\alpha_1$ being given twice the weight of $K\alpha_2$.

X-ray spectra



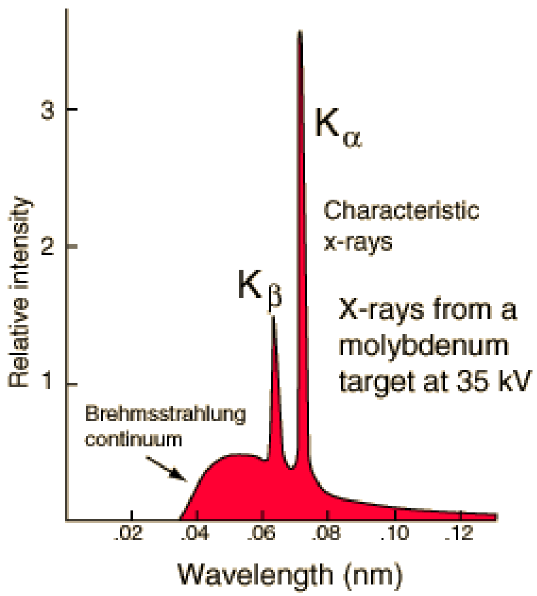


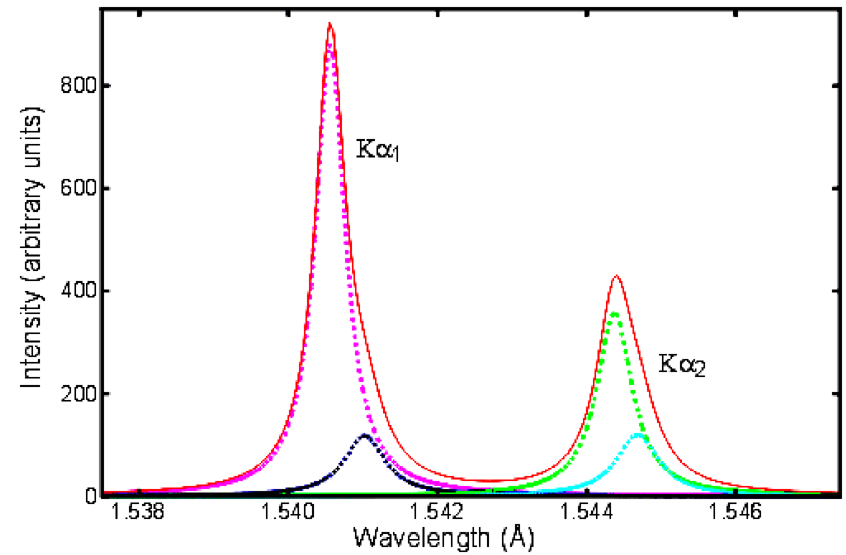
X-ray spectra

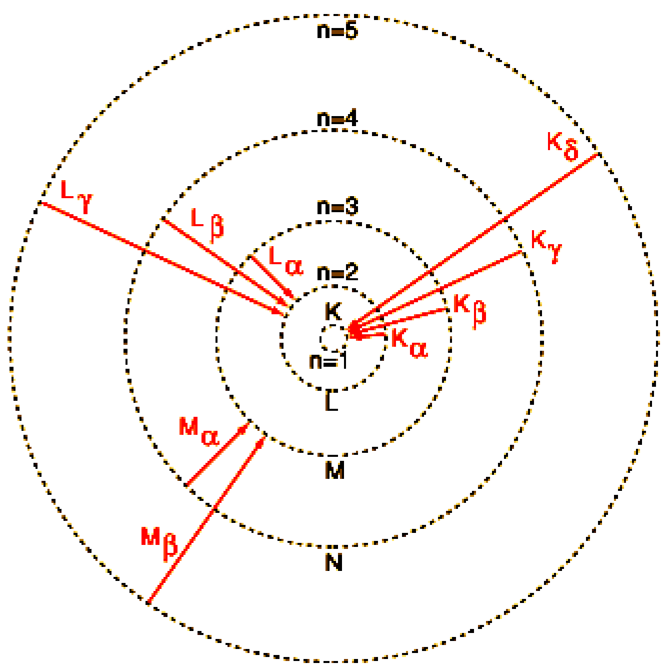
Experimental K-alpha x ray energies

Z	Element	$K\alpha_2$ eV(unc)	$K\alpha_1$ eV(unc)
10	Ne	848.61(26)	848.61(26)
11	Na	1040.98(12)	1040.98(12)
12	Mg	1253.437(13)	1253.688(11)
13	Al	1486.295(10)	1486.708(10)
14	Si	1739.394(34)	1739.985(19)
23	V	4944.671(59)	4952.216(59)
24	Cr	5405.5384(71)	5414.8045(71)
25	Mn	5887.6859(84)	5898.8010(84)
26	Fe	6391.0264(99)	6404.0062(99)
27	Co	6915.5380(39)	6930.3780(39)
28	Ni	7461.0343(45)	7478.2521(45)
29	Cu	8027.8416(26)	8047.8227(26)
30	Zn	8615.823(73)	8638.906(73)
31	Ga	9224.835(27)	9251.674(66)
32	Ge	9855.42(10)	9886.52(11)
39	Y	14882.94(26)	14958.54(27)
40	Zr	15690.645(50)	15774.914(54)
41	Nb	16521.28(33)	16615.16(33)
42	Mo	17374.29(29)	17479.372(10)
43	Tc	18250.9(12)	18367.2(12) *
44	Ru	19150.49(18)	19279.16(18)
45	Rh	20073.67(20)	20216.12(20)
46	Pd	21020.15(22)	21177.08(17)
47	Ag	21990.30(10)	22162.917(30)
48	Cd	22984.05(20)	23173.98(20)

X-ray spectra







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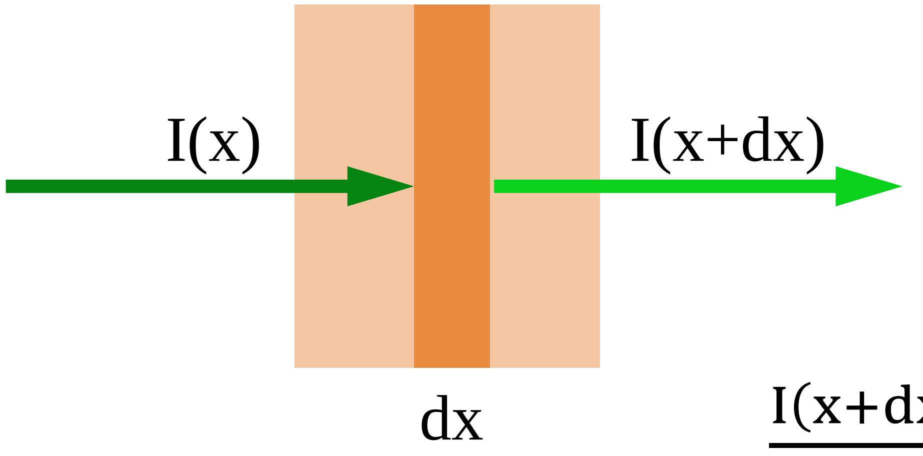

$$\frac{I(x+dx)-I(x)}{I(x)} = \frac{dI}{I} = -\mu dx$$

$$I_x = I_o e^{-\mu x} = I_o e^{-(\mu/\rho)\rho x}$$

μ/ρ : mass-absorption coefficient

$\mu/\rho = k\,\lambda^3\,Z^3$ between absorption edges

X-ray absorption spectrum for platinum

$$I = I_o e^{-\mu x} = I_o e^{-(\mu/\rho)\rho x}$$

μ/ρ : mass-absorption coefficient

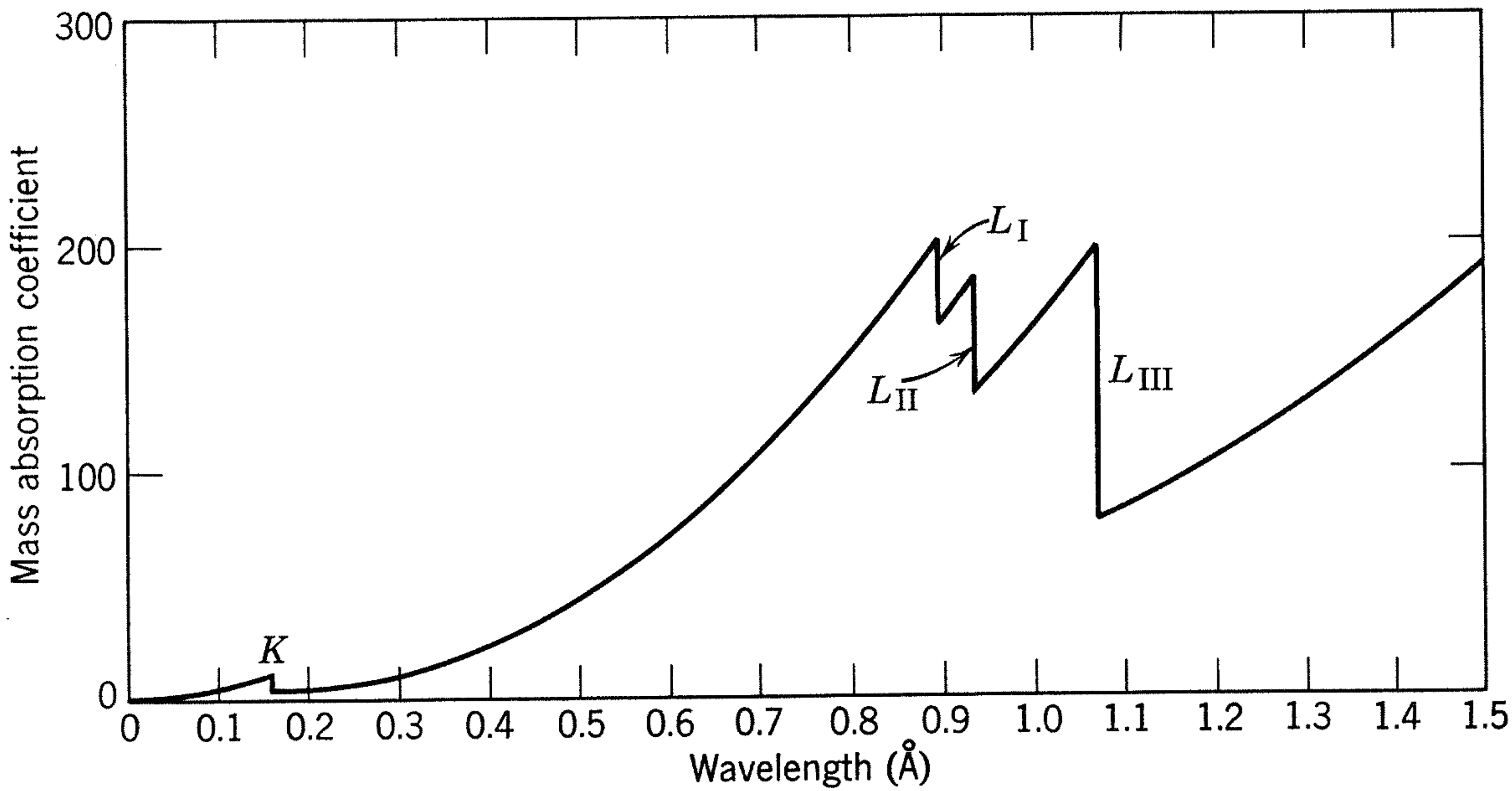

Fig. 2-19. Plot of the mass absorption coefficient for platinum versus wavelength, showing positions of the *K* and *L* absorption edges.

X-ray absorption

cm²/g

Appendix III

Mass Absorption Coefficients μ_m of the Elements ($Z = 1$ to 83) for a Selection of Wavelengths (Values given in italics are of low accuracy)

(Reprinted from *International Tables for X-Ray Crystallography*, Vol. III, with the permission of the Editorial Commission of the International Tables.)

Target radiation λ(A)		Ag Kα 0.5608	Ag Kβ₁ 0.4970	Rh Kα 0.6147	Rh Kβ₁ 0.5456	Mo Kα 0.7107	Mo Kβ₁ 0.6323	Cu Kα 1.5418	Cu Kβ₁ 1.3922	Co Kα 1.7902	Co Kβ₁ 1.6208	Fe Kα 1.9373	Fe Kβ₁ 1.7565	Cr Kα 2.2909	Cr Kβ₁ 2.0848	Ti Kα 2.7496	Ti Kβ₁ 2.5138
Absorber		μ_m (cm²/g)															
H	1	0.371	0.366	0.375	0.370	0.380	0.376	0.435	0.421	0.464	0.443	0.483	0.459	0.545	0.507	0.658	0.595
He	2	0.195	0.190	0.199	0.194	0.207	0.200	0.383	0.333	0.491	0.414	0.569	0.474	0.813	0.661	1.26	1.01
Li	3	0.187	0.177	0.197	0.185	0.217	0.200	0.716	0.571	1.03	0.804	1.25	0.978	1.96	1.52	3.26	2.53
Be	4	0.229	0.208	0.251	0.224	0.298	0.258	1.50	1.15	2.25	1.71	2.80	2.13	4.50	3.44	7.64	5.88
B	5	0.279	0.244	0.314	0.270	0.392	0.327	2.39	1.81	3.63	2.74	4.55	3.44	7.38	5.61	12.6	9.67
C	6	0.400	0.333	0.469	0.383	0.625	0.495	4.60	3.44	7.07	5.31	8.90	6.69	14.5	11.0	24.8	19.1
N	7	0.544	0.433	0.658	0.515	0.916	0.700	7.52	5.60	11.6	8.70	14.6	11.0	23.9	18.2	41.0	31.5
O	8	0.740	0.570	0.916	0.696	1.31	0.981	11.5	8.52	17.8	13.3	22.4	16.8	36.6	27.8	62.5	48.1
F	9	0.976	0.732	1.23	0.913	1.80	1.32	16.4	12.2	25.4	19.0	32.1	24.0	52.4	39.8	89.4	68.8
Ne	10	1.31	0.969	1.67	1.22	2.47	1.80	22.9	17.0	35.4	26.5	44.6	33.5	72.8	55.3	124	95.4
Na	11	1.67	1.22	2.15	1.56	3.21	2.32	30.1	22.3	46.5	34.8	58.6	44.0	95.3	72.5	162	125
Mg	12	2.12	1.54	2.73	1.97	4.11	2.96	38.6	28.7	59.5	44.6	74.8	56.3	121	92.4	204	158
Al	13	2.65	1.90	3.42	2.45	5.16	3.71	48.6	36.2	74.8	56.2	93.9	70.9	152	116	255	198
Si	14	3.28	2.35	4.25	3.04	6.44	4.61	60.6	45.1	93.3	70.1	117	88.3	189	144	315	245
P	15	4.01	2.85	5.20	3.71	7.89	5.64	74.1	55.2	114	85.5	142	108	229	175	381	297
S	16	4.84	3.44	6.29	4.48	9.55	6.82	89.1	66.5	136	103	170	129	272	209	450	352
Cl	17	5.77	4.09	7.51	5.34	11.4	8.14	106	79.0	161	122	200	152	318	246	522	410
A	18	6.81	4.82	8.87	6.29	13.5	9.62	123	92.4	187	142	232	177	366	284	593	469
K	19	8.00	5.66	10.4	7.39	15.8	11.3	143	107	215	164	266	204	417	325	667	531
Ca	20	9.28	6.57	12.1	8.58	18.3	13.1	162	122	243	186	299	231	463	363	728	585
Sc	21	10.7	7.57	13.9	9.89	21.1	15.1	184	139	273	210	336	260	513	405	794	643
Ti	22	12.3	8.70	16.0	11.4	24.2	17.3	208	158	308	237	377	293	571	453	98.4	75.8
V	23	14.0	9.91	18.2	12.9	27.5	19.7	233	178	343	266	419	327	68.4	502	116	89.6
Cr	24	15.8	11.2	20.6	14.6	31.1	22.3	260	199	381	296	463	363	79.8	60.7	135	104
Mn	25	17.7	12.6	23.0	16.4	34.7	24.9	285	219	414	323	57.2	395	93.0	70.8	157	122

Warren, X-ray diffraction

X-ray absorption

cm²/g

Target radiation λ(A)		Ag $K\bar{\alpha}$ 0.5608	Ag $K\beta_1$ 0.4970	Rh $K\bar{\alpha}$ 0.6147	Rh $K\beta_1$ 0.5456	Mo $K\bar{\alpha}$ 0.7107	Mo $K\beta_1$ 0.6323	Cu $K\bar{\alpha}$ 1.5418	Cu $K\beta_1$ 1.3922	Co $K\bar{\alpha}$ 1.7902	Co $K\beta_1$ 1.6208	Fe $K\bar{\alpha}$ 1.9373	Fe $K\beta_1$ 1.7565	Cr $K\bar{\alpha}$ 2.2909	Cr $K\beta_1$ 2.0848	Ti $K\bar{\alpha}$ 2.7496	Ti $K\beta_1$ 2.5138
Fe	26	19.7	14.0	25.6	18.2	38.5	27.7	308	238	52.8	349	66.4	50.0	108	82.2	182	141
Co	27	21.8	15.5	28.3	20.2	42.5	30.6	313	257	61.1	45.8	76.8	57.8	125	95.0	210	163
Ni	28	24.1	17.1	31.1	22.3	46.6	33.7	45.7	275	70.5	52.8	88.6	66.7	144	109	242	187
Cu	29	26.4	18.8	34.1	24.4	50.9	36.9	52.9	39.3	81.6	61.2	103	77.3	166	127	280	217
Zn	30	28.8	20.6	37.2	26.7	55.4	40.2	60.3	44.8	93.0	69.7	117	88.0	189	144	318	246
Ga	31	31.4	22.4	40.4	29.1	60.1	43.7	67.9	50.5	105	78.4	131	98.9	212	162	356	276
Ge	32	34.1	24.4	43.8	31.6	64.8	47.3	75.6	56.2	116	87.3	146	110	235	180	393	306
As	33	36.9	26.5	47.3	34.2	69.7	51.1	83.4	62.1	128	96.2	160	121	258	198	430	335
Se	34	39.8	28.6	50.9	36.9	74.7	54.9	91.4	68.1	140	105	175	133	281	216	467	364
Br	35	42.7	30.8	54.6	39.7	79.8	58.8	99.6	74.4	152	115	190	144	305	234	503	394
Kr	36	45.8	33.1	58.3	42.5	84.9	62.8	108	80.7	165	124	206	156	327	252	538	422
Rb	37	48.9	35.4	62.2	45.5	90.0	66.9	117	87.3	177	134	221	168	351	271	573	451
Sr	38	52.1	37.8	66.0	48.4	95.0	70.9	125	94.0	190	144	236	180	373	289	606	479
Y	39	55.3	40.3	69.9	51.5	100	75.0	134	101	203	154	252	193	396	308	638	506
Zr	40	58.5	42.8	73.7	54.5	15.9	79.0	143	108	216	165	268	205	419	326	669	533
Nb	41	61.7	45.3	77.4	57.5	17.1	82.9	153	115	230	175	284	218	441	345	699	559
Mo	42	64.8	47.8	81.1	60.5	18.4	13.1	162	123	243	186	300	231	463	363	727	584
Tc	43	67.9	50.3	13.0	63.5	19.7	14.1	172	131	257	197	316	244	485	382	753	609
Ru	44	10.7	52.8	13.9	66.4	21.1	15.1	183	139	272	209	334	259	509	403	784	637
Rh	45	11.5	55.2	14.9	10.6	22.6	16.2	194	148	288	222	352	274	534	424	814	665
Pd	46	12.3	57.5	15.9	11.3	24.1	17.3	206	157	304	235	371	289	559	446	845	694
Ag	47	13.1	9.29	17.0	12.1	25.8	18.5	218	166	321	248	391	305	586	468	876	723
Cd	48	14.0	9.91	18.2	12.9	27.5	19.7	231	176	338	262	412	322	613	492	908	753
In	49	14.9	10.6	19.4	13.8	29.3	21.0	243	186	356	277	432	339	638	514	935	781
Sn	50	15.9	11.3	20.6	14.7	31.1	22.3	256	197	373	291	451	356	662	536	957	805
Sb	51	16.9	12.0	21.9	15.6	33.1	23.8	270	207	391	306	472	373	688	559	1100	832
Te	52	17.9	12.7	23.3	16.6	35.0	25.2	282	218	407	320	490	389	707	578	557	899
I	53	19.0	13.5	24.6	17.6	37.1	26.7	294	228	422	333	506	404	722	594	214	919
Xe	54	20.1	14.3	26.1	18.6	39.2	28.2	306	238	436	346	521	418	763	609	245	511
Cs	55	21.3	15.1	27.5	19.7	41.3	29.8	318	248	450	358	534	431	793	621	274	215

Warren, X-ray diffraction

X-ray absorption

cm^2/g

Target radiation		Ag		Rh		Mo		Cu		Co		Fe		Cr		Ti	
		$K\bar{\alpha}$	$K\beta_1$	$K\bar{\alpha}$	$K\beta_1$	$K\bar{\alpha}$	$K\beta_1$	$K\bar{\alpha}$	$K\beta_1$	$K\bar{\alpha}$	$K\beta_1$	$K\bar{\alpha}$	$K\beta_1$	$K\bar{\alpha}$	$K\beta_1$	$K\bar{\alpha}$	$K\beta_1$
λ(Å)		0.5608	0.4970	0.6147	0.5456	0.7107	0.6323	1.5418	1.3922	1.7902	1.6208	1.9373	1.7565	2.2909	2.0848	2.7496	2.5138
Absorber		μ_m (cm^2/g)															
Ba	56	22.5	16.0	29.1	20.8	43.5	31.4	330	258	463	370	546	444	461	661	302	237
La	57	23.7	16.9	30.6	21.9	45.8	33.2	341	268	475	382	557	456	202	681	329	259
Ce	58	25.0	17.8	32.3	23.1	48.2	34.9	352	278	486	394	601	468	219	409	356	281
Pr	59	26.3	18.8	34.0	24.4	50.7	36.7	363	288	497	405	359	479	236	183	381	302
Nd	60	27.7	19.8	35.7	25.7	53.2	38.6	374	298	543	416	379	519	252	196	405	322
Pm	61	29.1	20.8	37.6	27.0	55.9	40.6	386	308	327	428	172	538	268	209	429	342
Sm	62	30.6	21.9	39.5	28.4	58.6	42.6	397	319	344	461	182	328	284	222	452	361
Eu	63	32.2	23.0	41.4	29.8	61.5	44.8	425	329	156	478	193	344	299	234	473	379
Gd	64	33.8	24.2	43.5	31.3	64.4	47.0	439	340	165	295	203	157	314	247	495	397
Tb	65	35.5	25.4	45.6	32.9	67.5	49.2	273	352	173	309	214	165	329	259	516	415
Dy	66	37.2	26.6	47.8	34.5	70.6	51.6	286	369	182	140	224	173	344	271	536	433
Ho	67	39.0	27.9	50.0	36.1	73.9	54.0	128	231	191	146	234	181	359	283	555	450
Er	68	40.8	29.3	52.4	37.9	77.3	56.6	134	242	199	153	245	190	373	295	574	466
Tm	69	42.8	30.7	54.9	39.7	80.8	59.2	140	252	208	160	255	198	387	307	592	483
Yb	70	44.8	32.2	57.4	41.5	84.5	61.9	146	111	217	167	265	206	401	319	610	499
Lu	71	46.8	33.6	60.0	43.4	88.2	64.7	153	116	226	174	276	215	416	331	628	515
Hf	72	48.8	35.1	62.5	45.3	91.7	67.4	159	121	235	181	286	223	430	343	645	532
Ta	73	50.9	36.7	65.1	47.3	95.4	70.2	166	126	244	189	297	232	444	355	662	547
W	74	53.0	38.2	67.8	49.3	99.1	73.1	172	132	253	196	308	241	458	368	679	563
Re	75	55.2	39.8	70.4	51.2	103	75.9	179	137	262	204	319	250	473	380	696	579
Os	76	57.3	41.4	73.1	53.2	106	78.7	186	143	272	212	330	259	487	393	712	595
Ir	77	59.4	42.9	75.6	55.2	110	81.4	193	148	282	219	341	269	502	406	729	611
Pt	78	61.4	44.5	78.0	57.1	113	83.9	200	154	291	228	353	278	517	419	745	628
Au	79	63.1	45.8	80.0	58.7	115	86.0	208	160	302	236	365	288	532	432	761	644
Hg	80	64.7	47.1	81.8	60.2	117	87.9	216	166	312	245	377	298	547	446	777	660
Tl	81	66.2	48.4	83.5	61.7	119	89.5	224	172	323	253	389	309	563	460	794	677
Pb	82	67.7	49.8	85.0	63.2	120	91.0	232	179	334	262	402	319	579	474	810	694
Bi	83	69.1	51.1	86.1	64.6	120	92.0	240	185	346	272	415	330	596	489	827	712

Warren, X-ray diffraction

X-ray filters

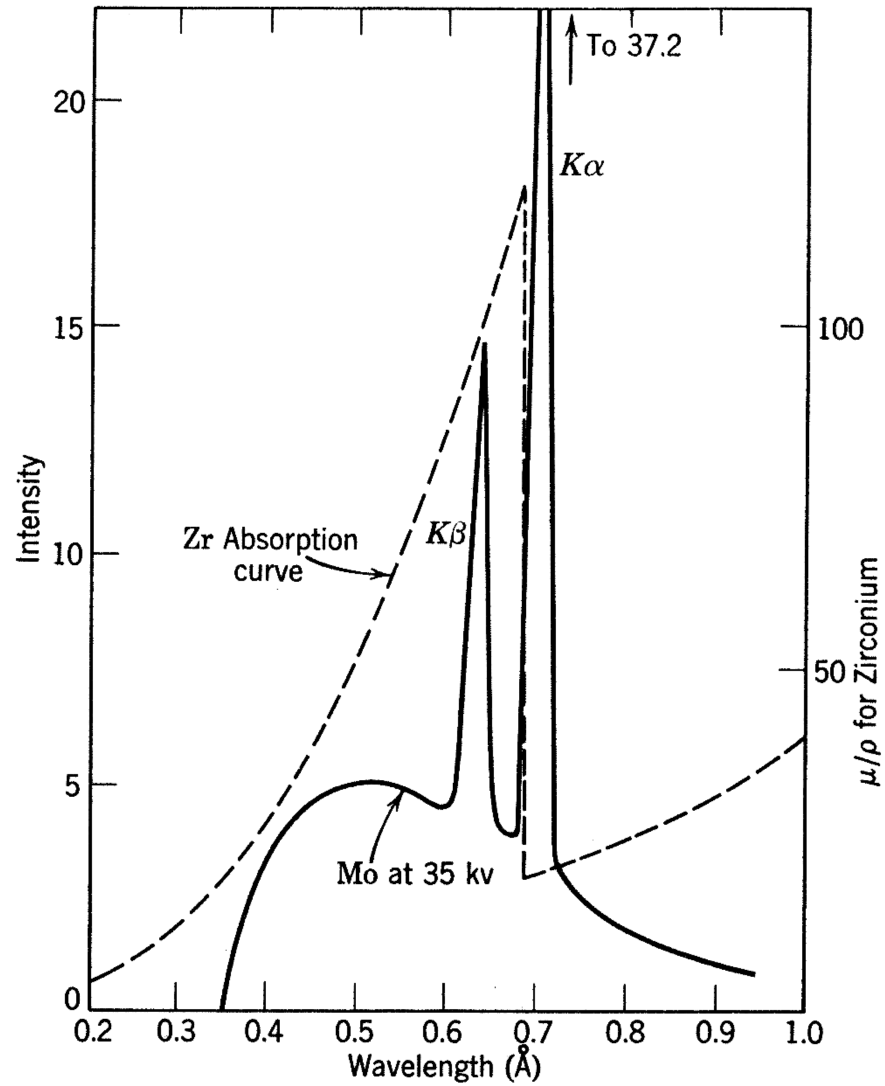

Fig. 2-20. The zirconium absorption curve superposed on 35-kV molybdenum radiation.

Fundamentals of X-ray scattering

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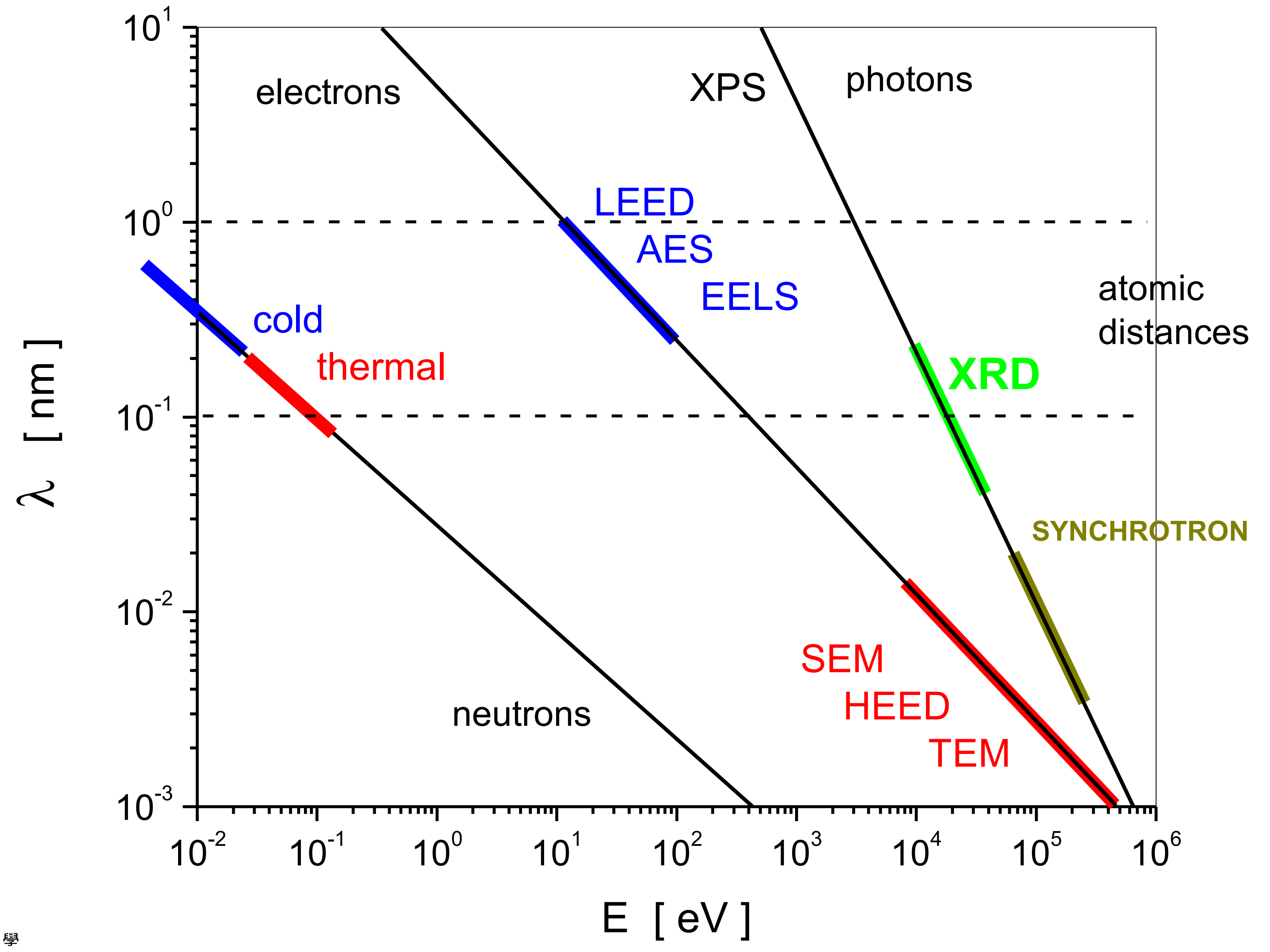
Darwin-breadth (qualitatively)

Monochromators (briefly)

correspondence between different radiations



correspondence between different radiations

Properties	electrons	X-rays	neutrons
charge	e	0	0
rest-mass	m	0	M
λ	$h/\sqrt{2mE}$=0.123 nm$\sqrt{eV}$ $\times\sqrt{E+10^{-6}E^2}$	hc/E= 1240 nm eV /E	$h/\sqrt{2ME}$= 3.08 nm $/\sqrt{T(K)}$
interaction	Coulomb	electrodynamic	nuclear + magnetic
Energy range	10 eV – 400 keV	2 keV – 200 keV	10 meV - eV
absorption length	0.1 nm – 200 nm	1 nm – 10 mm	≥ 1 mm
scattering-length	0.1 nm	-3×10^{-14} m	$\pm1\times10^{-14}$ m

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solving the acronyms

LEED: low energy electron diffraction

AES: Auger electron scattering

EELS: electron energy loss spectroscopy

SEM: scanning electron microscopy

HEED: high energy electron diffraction

TEM: transmission electron microscopy

XRD: X-ray diffraction

Cold/thermal: thermalized neutrons

XPS: X-ray-photon-spectroscopy

Synchrotron: synchrotron source of ***photons***

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The first ”synchrotron source”

“Synchrotron radiation was seen for the first time at the General Electric in the USA in 1947”

Brilliance of X-ray sources:

$$\frac{\text{number of fotons}}{\text{sec} \times \text{mm}^2}$$

foton/s/mm^2

10^{34}

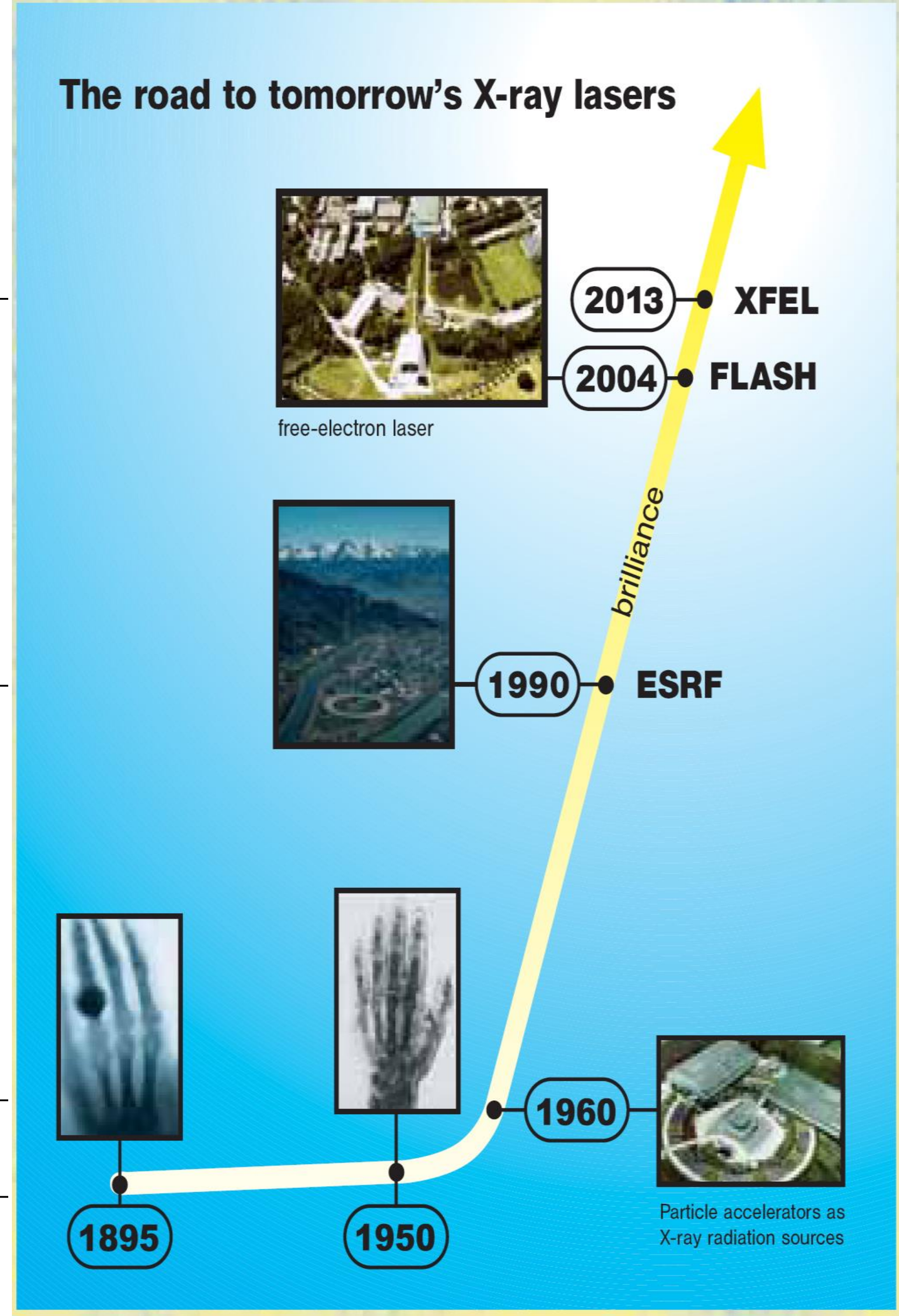
10^{24}

10^{12}

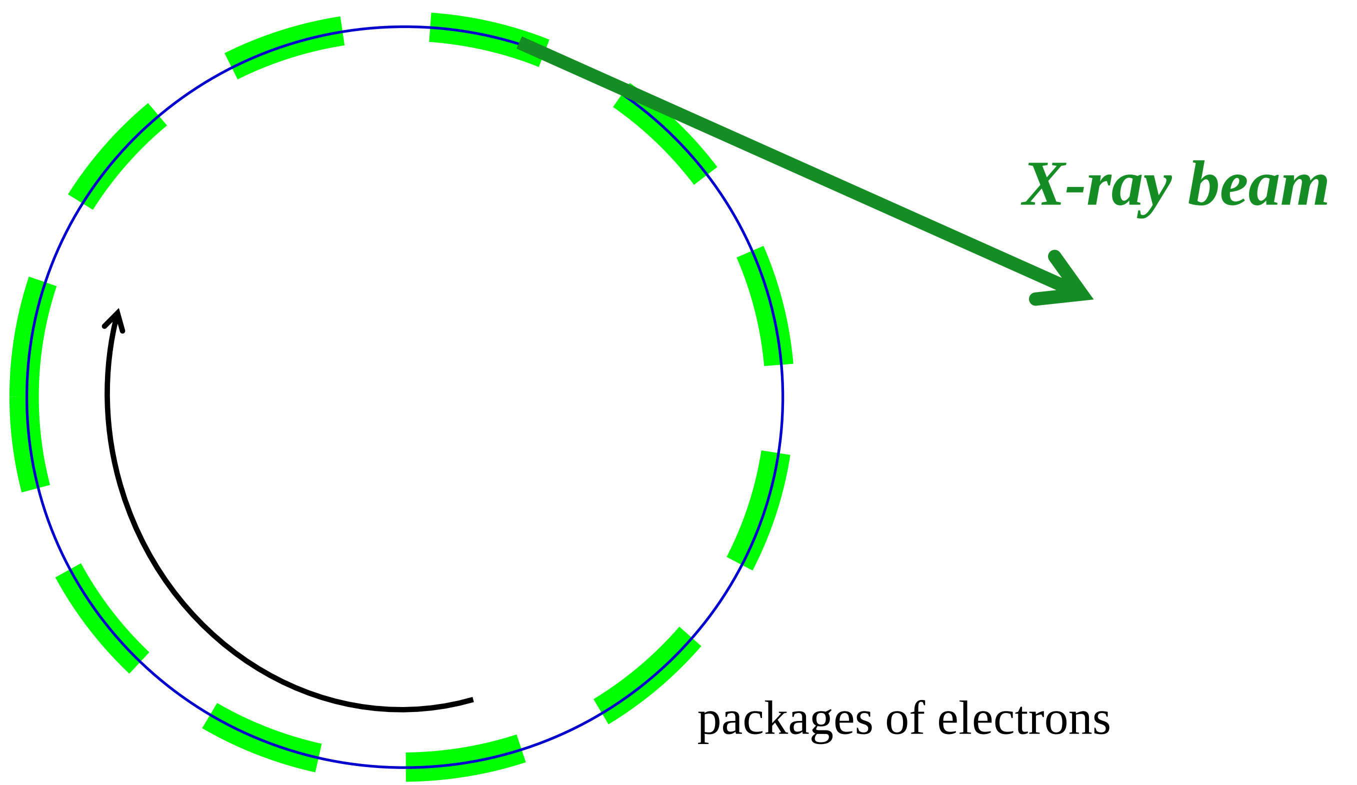
10^{8}

120 years of

brilliance



Synchrotron X-ray sources

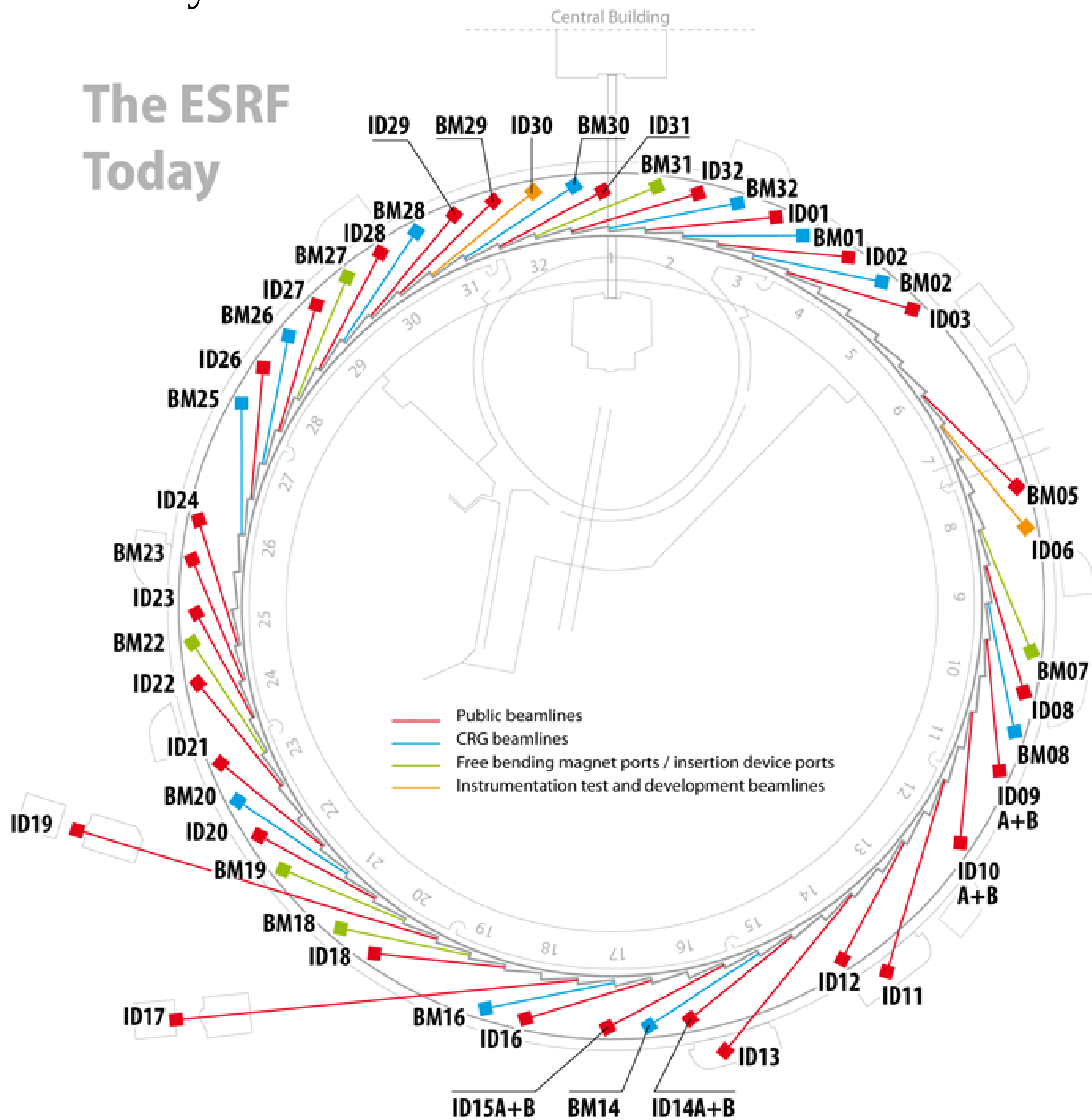


ESRF, Grenoble

European Synchrotron Radiation Facility

ESRF, Grenoble

European Synchrotron Radiation Facility

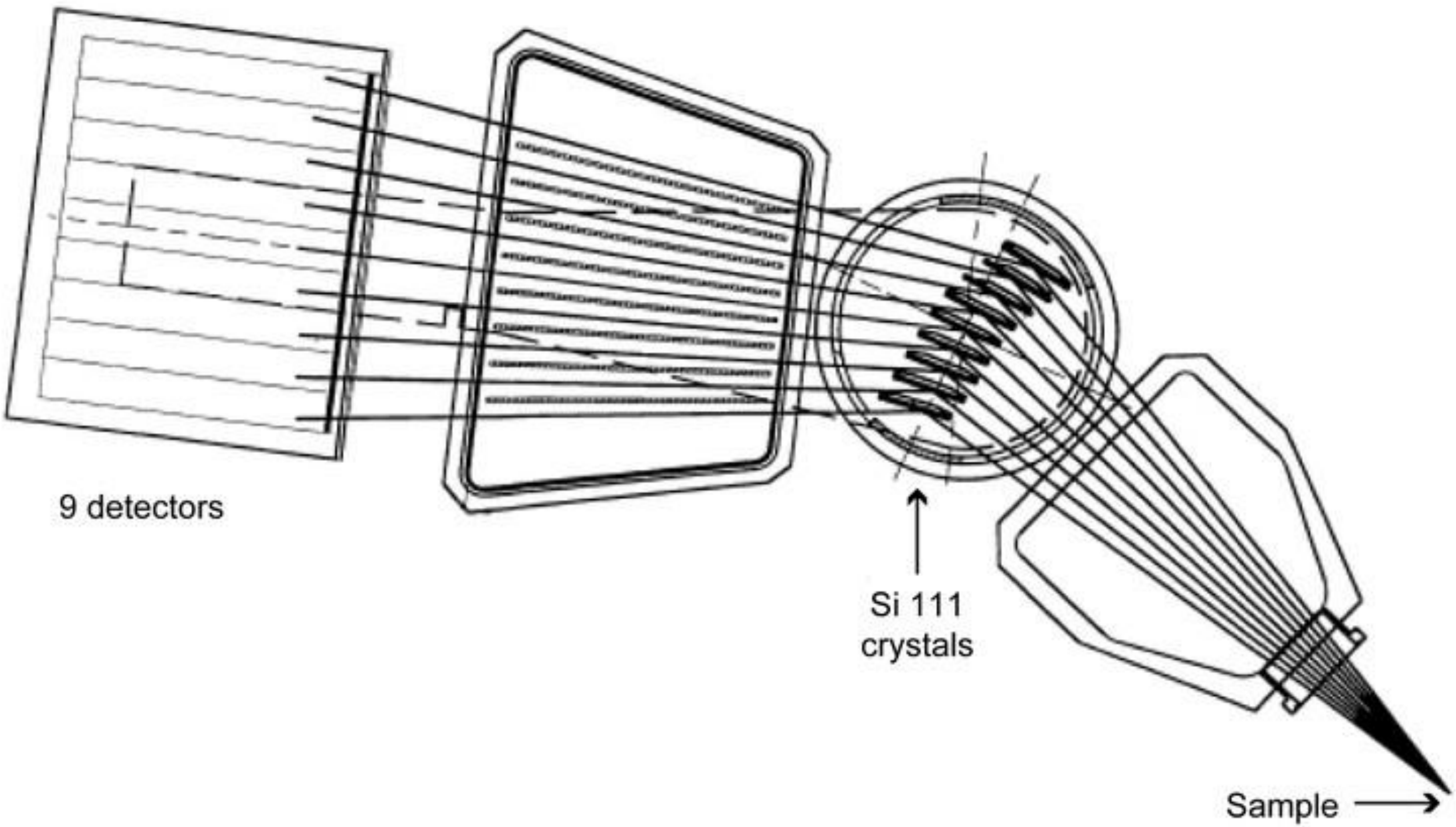


ID31

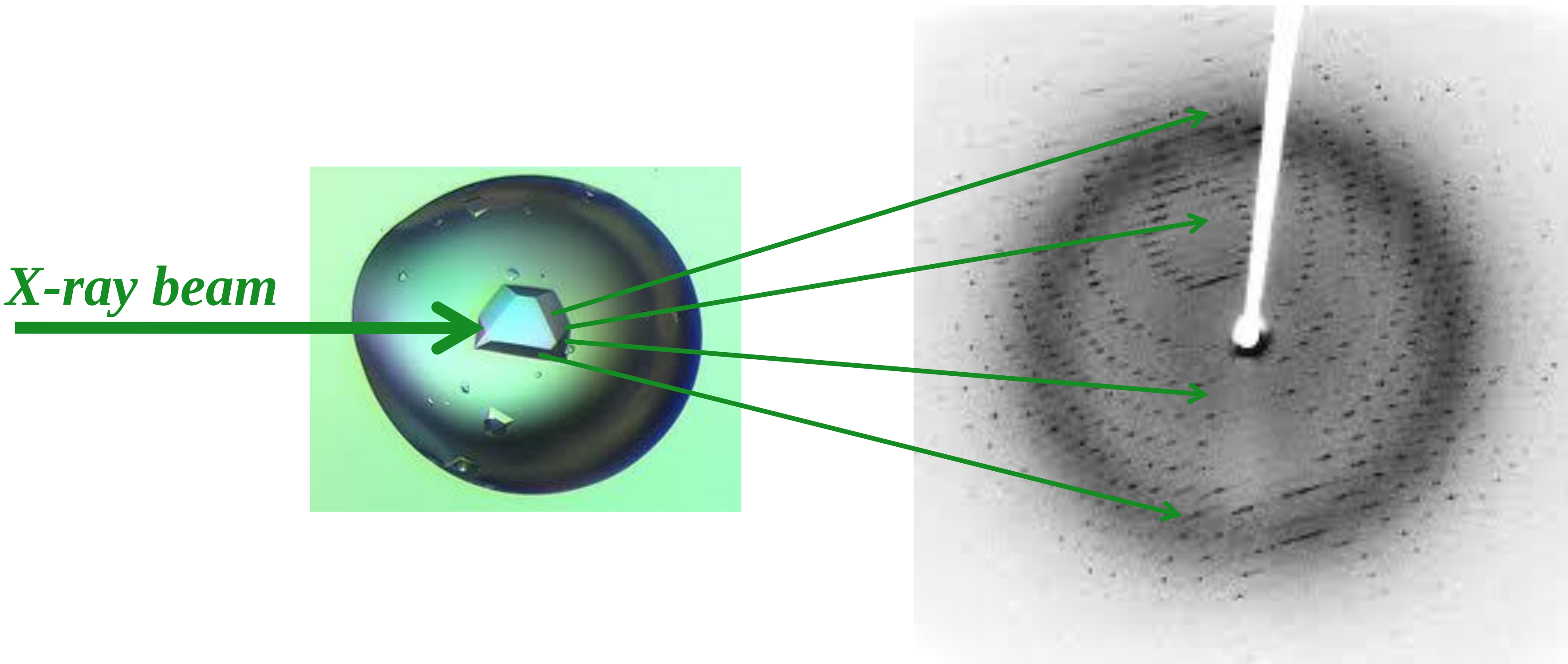
high resolution
powder diffractometer

~ 3 m

ID31 high resolution powder diffractometer: detector system



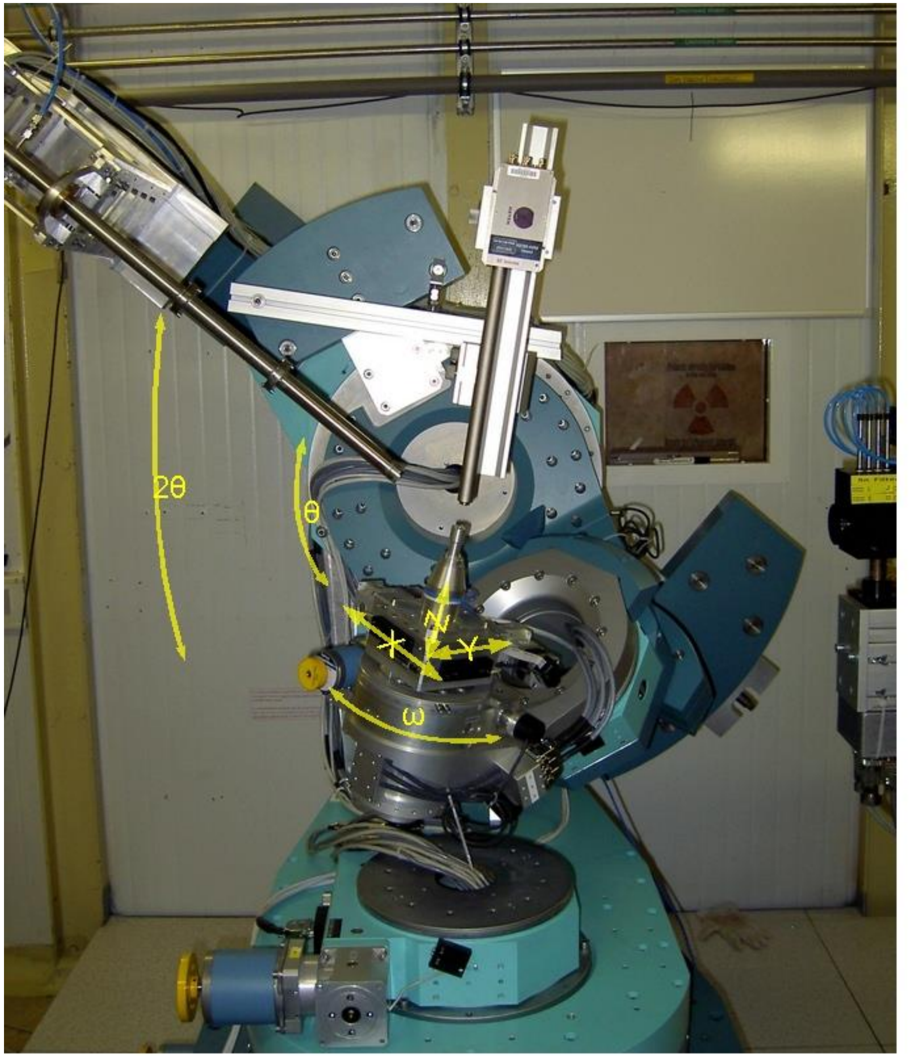
protein crystallography



protein crystallography

ESRF, Grenoble

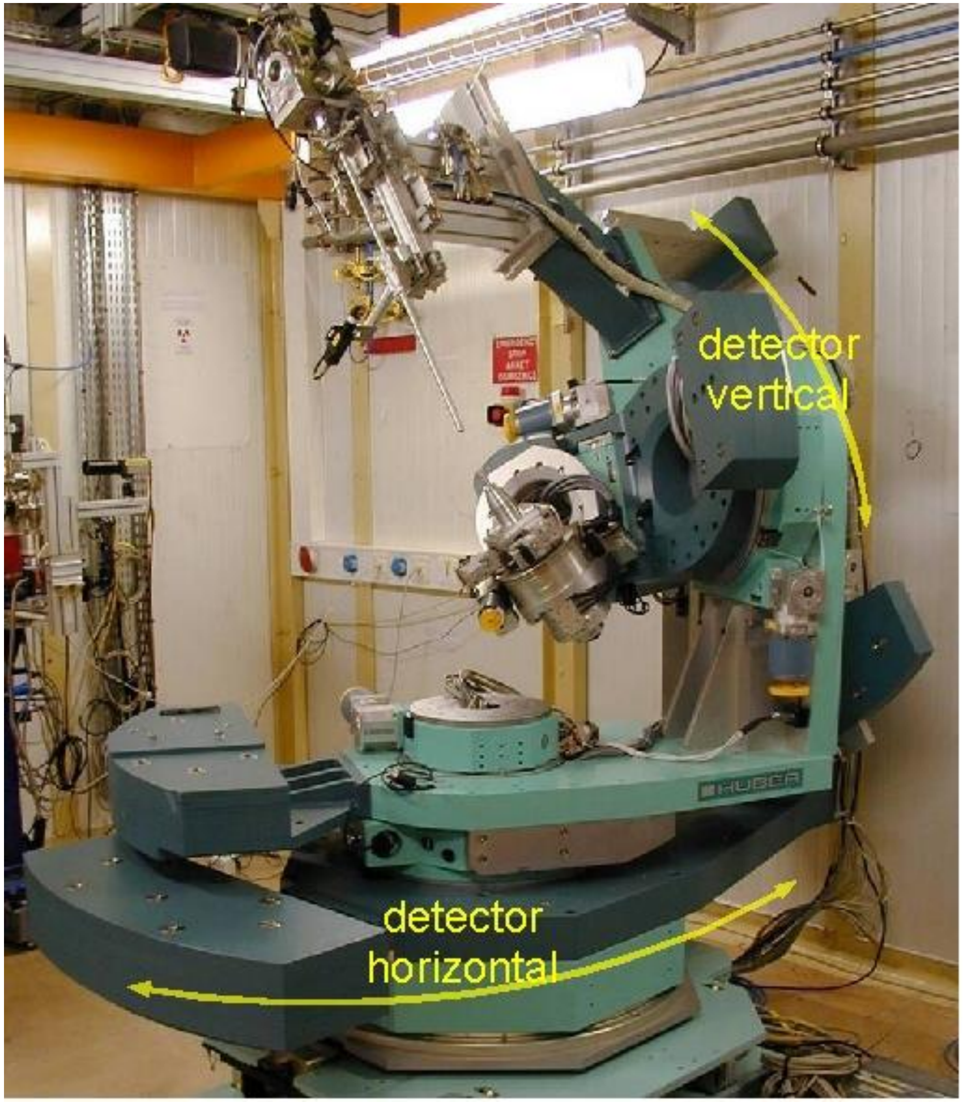
European Synchrotron Radiation Facility



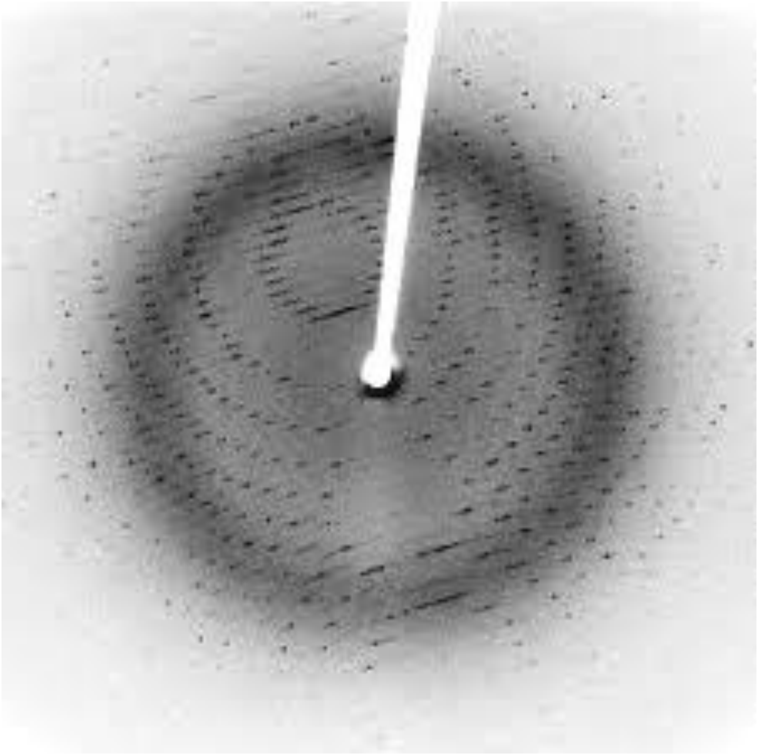
protein crystallography

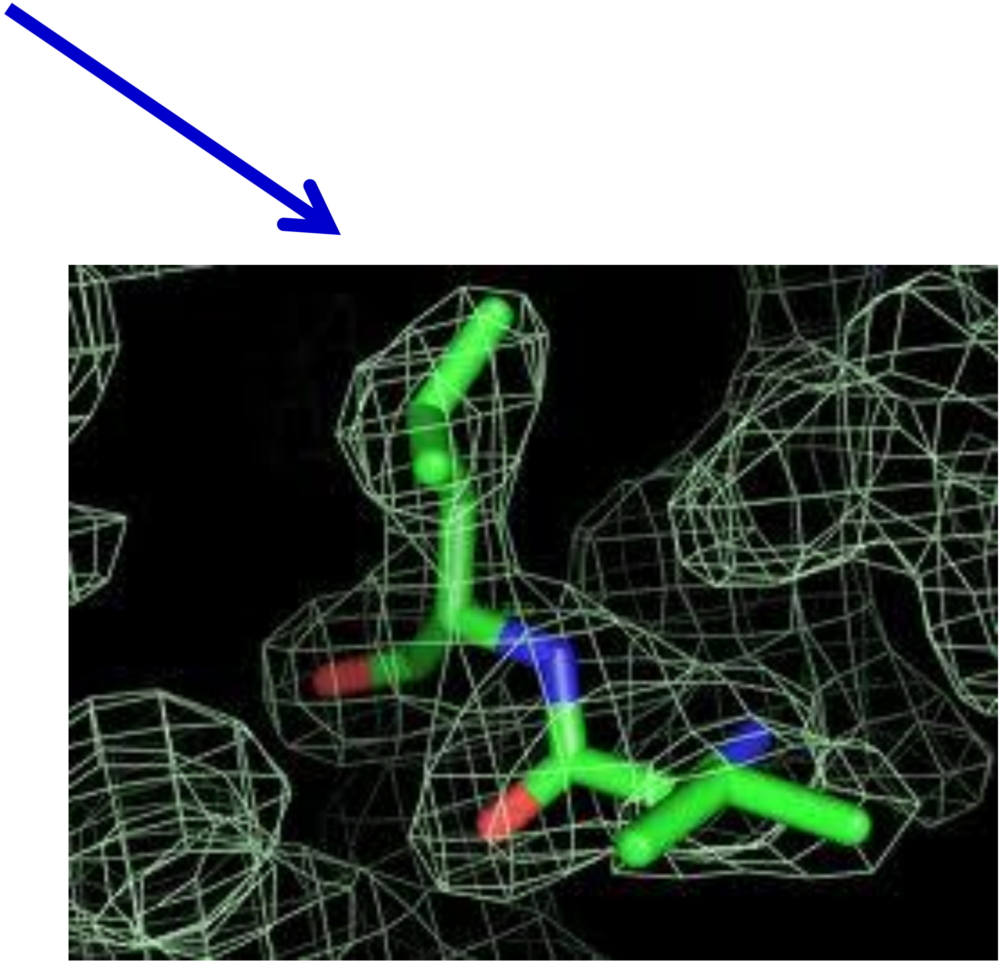
ESRF, Grenoble

European Synchrotron Radiation Facility



protein crystallography





APS, Argonne, IL, USA

Advanced Photon Source

SPring-8

Japan's synchrotron

SPring-8

Japan's synchrotron

controlling the path of electrons

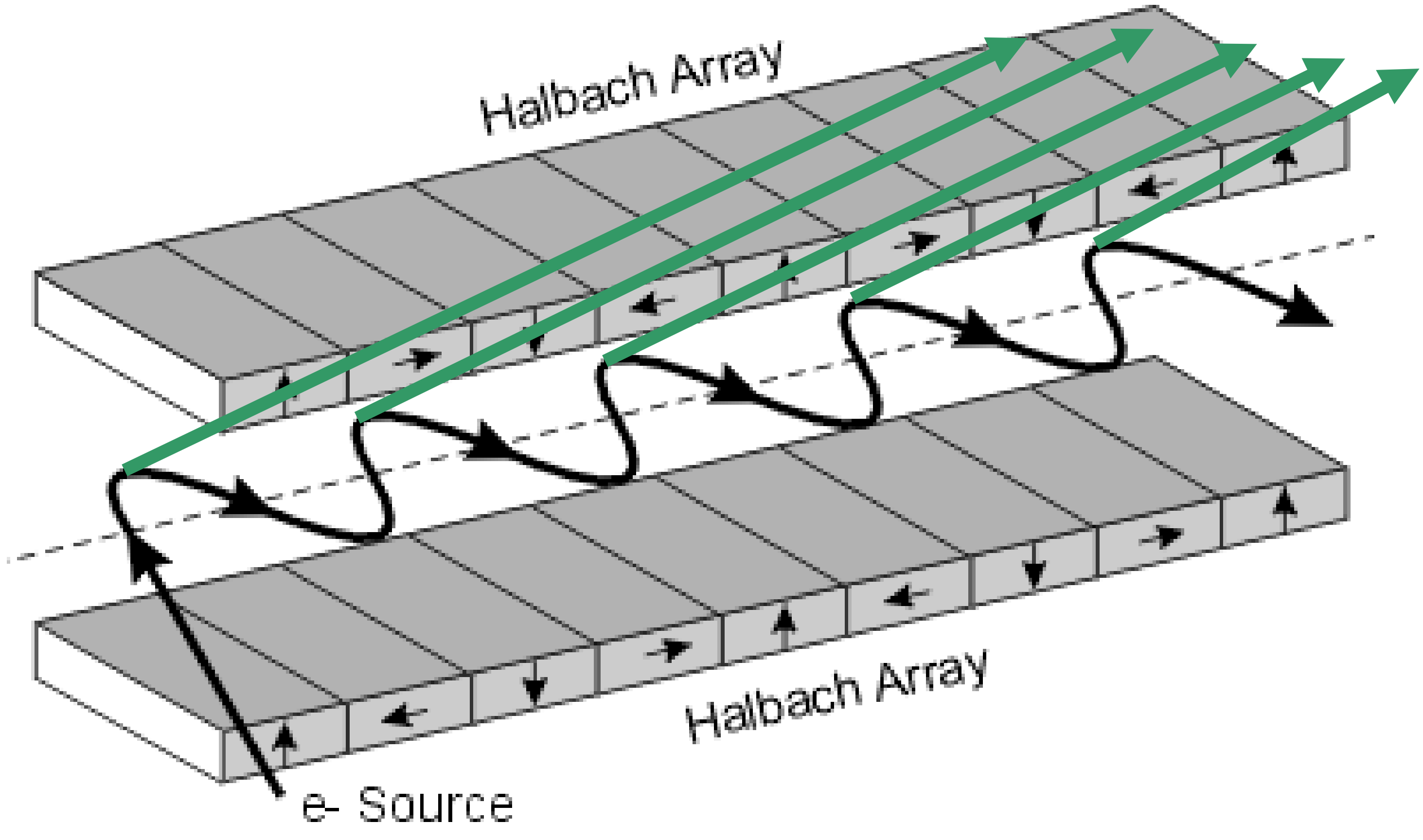
incertion devices

- Bending magnet
- Wiggler
- Undulator

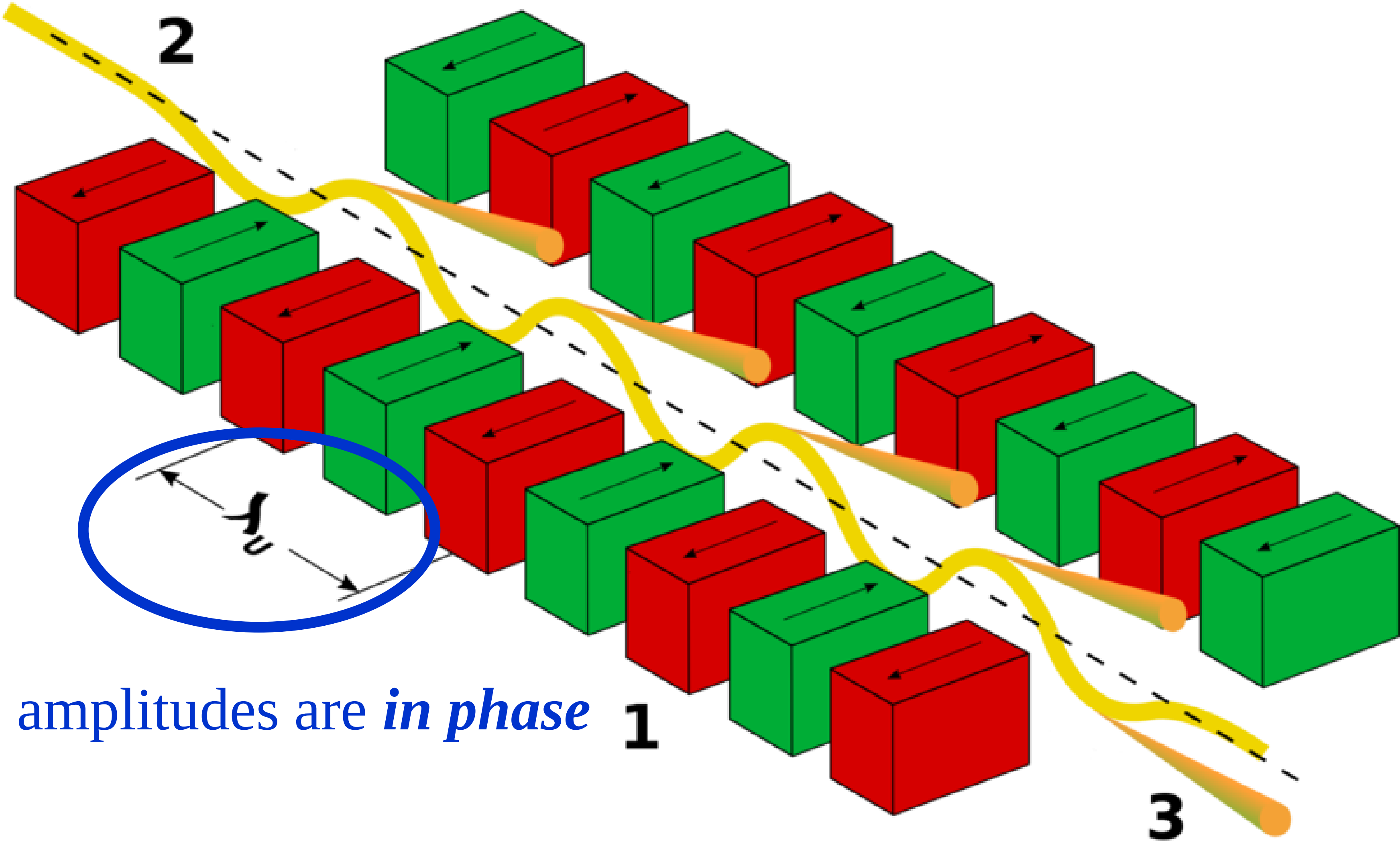
Bending magnet

Wiggler

Intensities are adding up

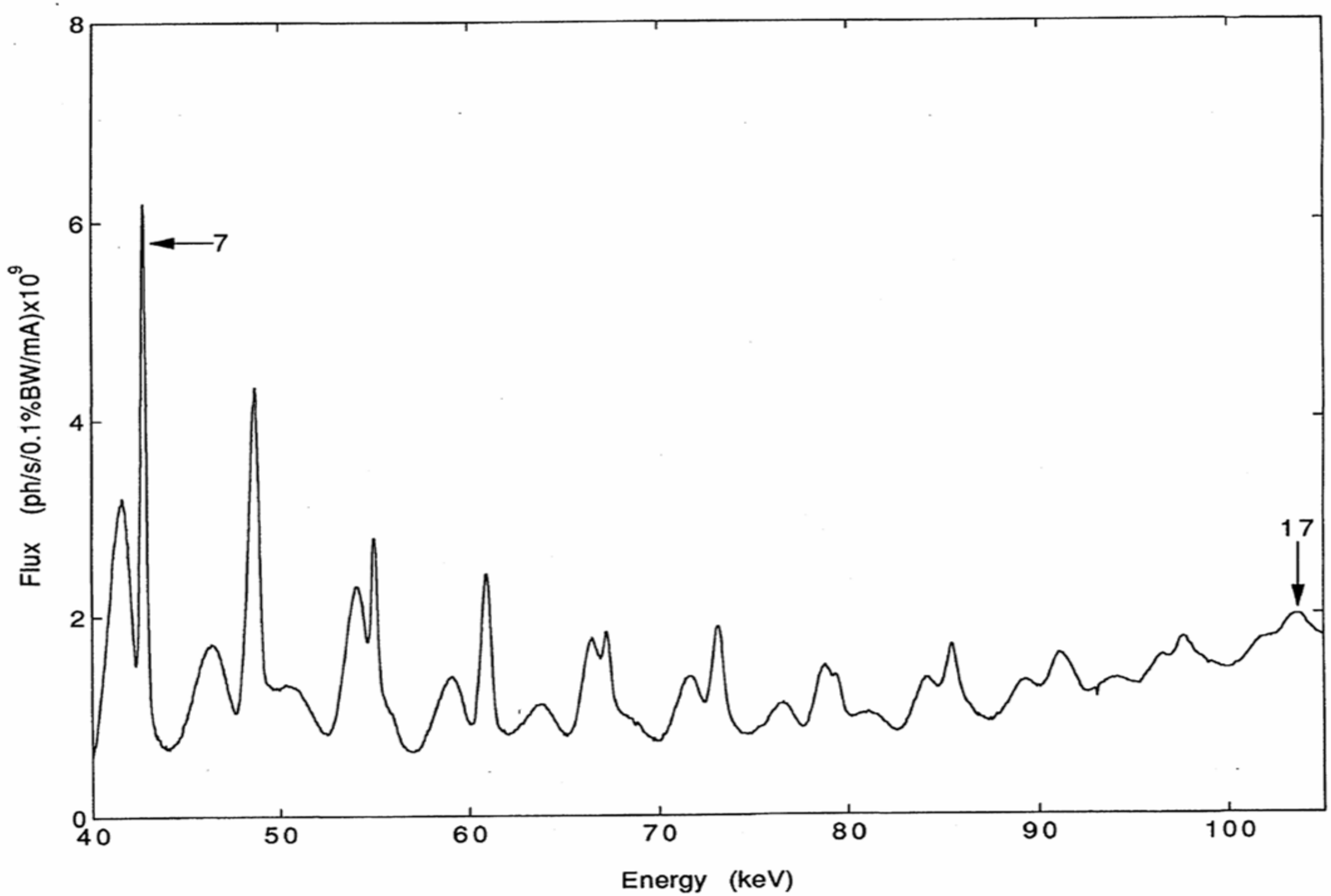


Undulator



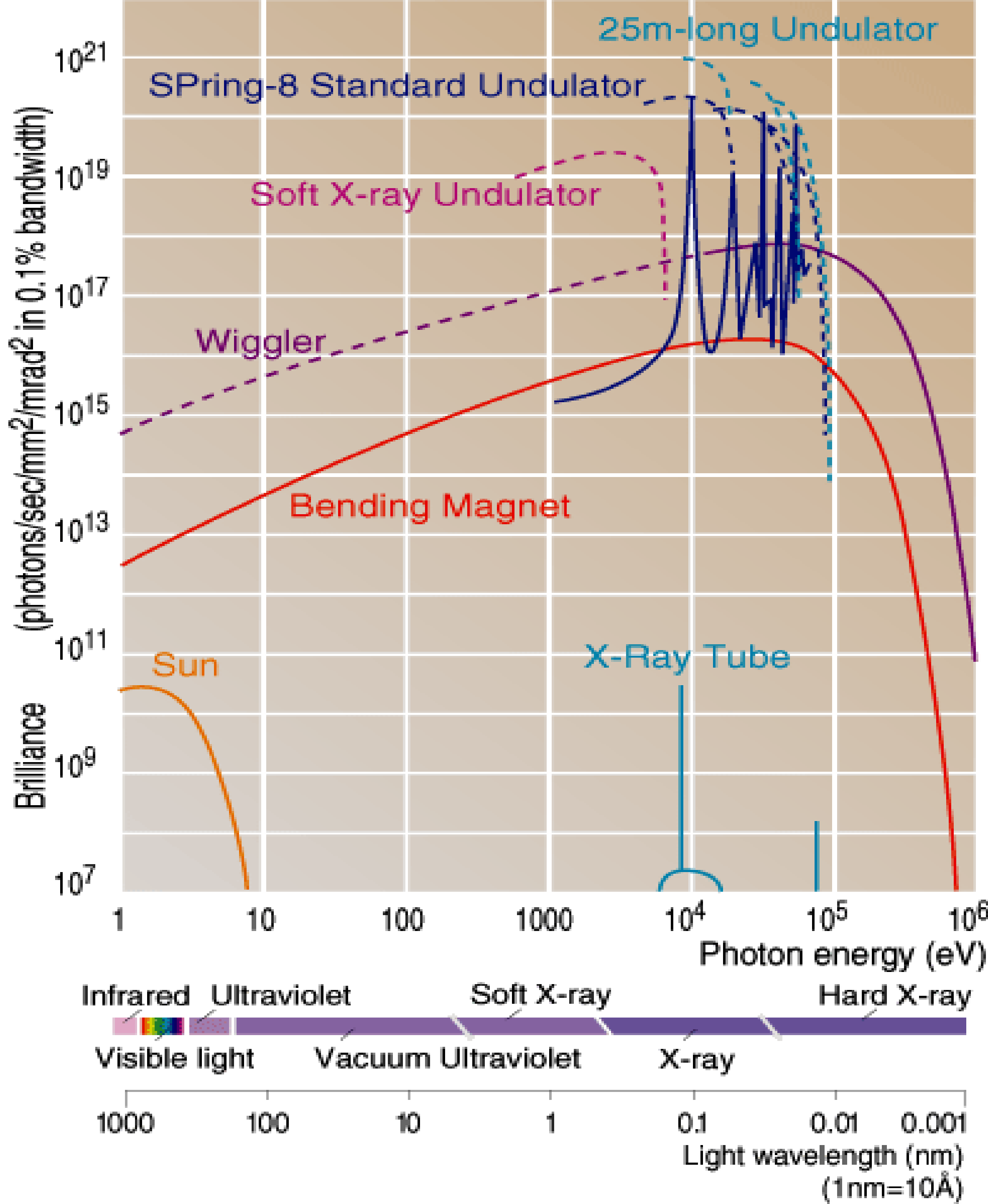
the amplitudes are ***in phase***

typical **undulator** spectrum at ***APS - Argonne***



X-ray spectra at

SPring-8

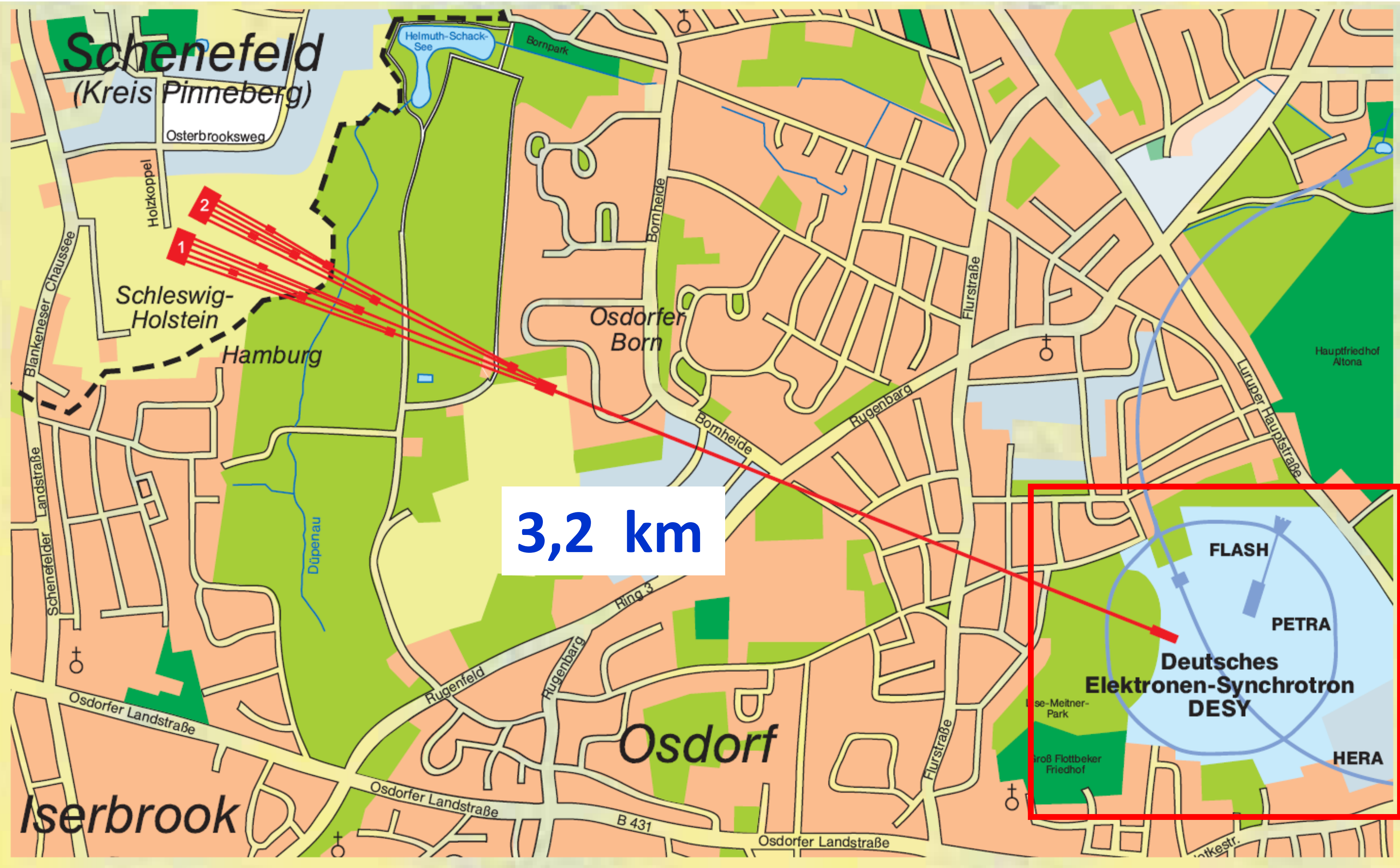


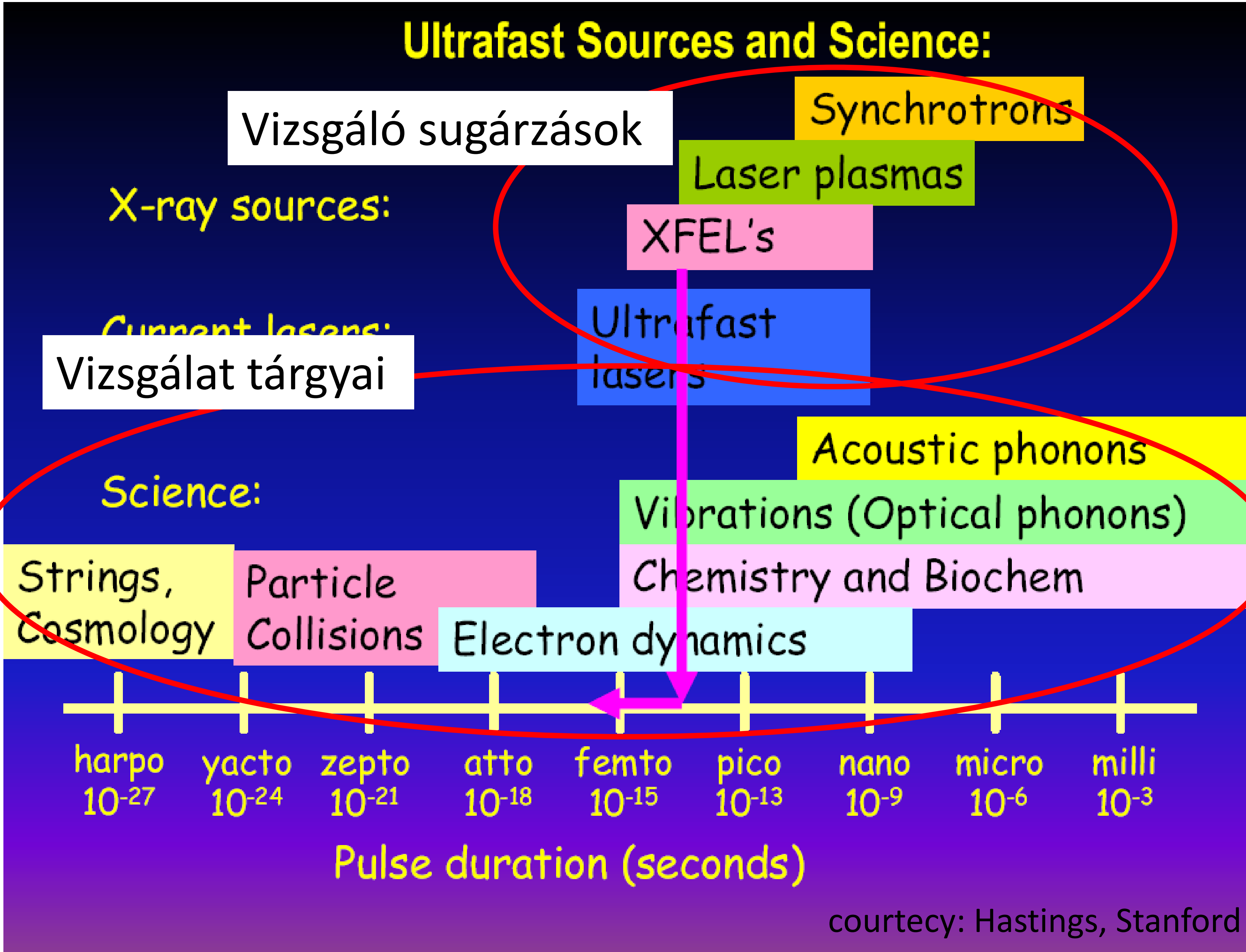
free electron laser: FEL

a very long undulator

the synchrotron in Hamburg (Germany) today:

schematics of the European Free Electron Laser (XFEL)





Ultrafast Sources and Science:
Vizsgáló sugárzások
Synchrotrons
Laser plasmas
X-ray sources:
XFEL's
Current lasers:
Ultrafast lasers
Vizsgálat tárgyai
Acoustic phonons
Science:
Vibrations (Optical phonons)
Chemistry and Biochem
Strings, Cosmology
Particle Collisions
Electron dynamics
harpo 10^{-27}
yacto 10^{-24}
zepto 10^{-21}
atto 10^{-18}
femto 10^{-15}
pico 10^{-13}
nano 10^{-9}
micro 10^{-6}
milli 10^{-3}
Pulse duration (seconds)
courtecy: Hastings, Stanford

prospective diffraction on

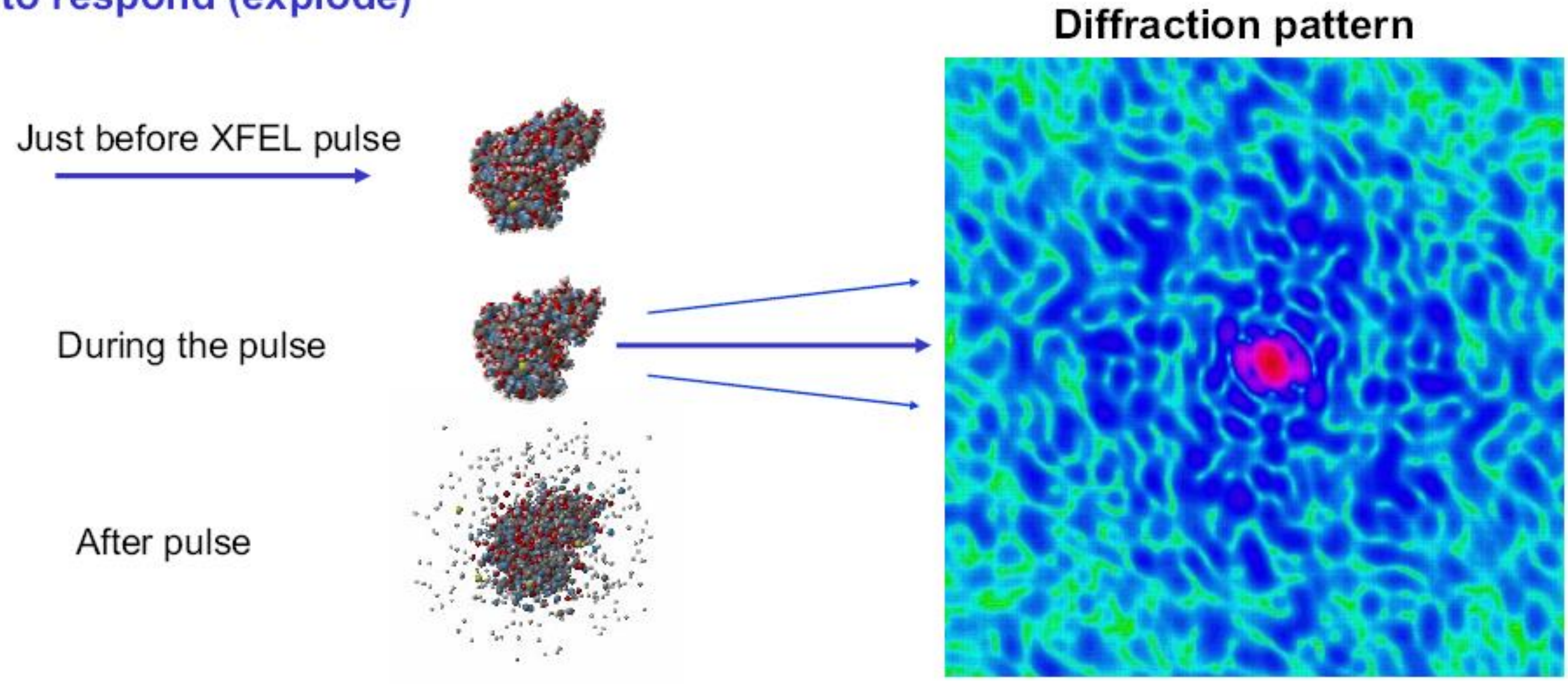
single molecules

at the European FEL

THEORY predicts XFELs may allow high resolution imaging of single particles / molecules

Neutze, Wouts, van der Spoel, Weckert, Hajdu *Nature* 406, 752-757 (2000)

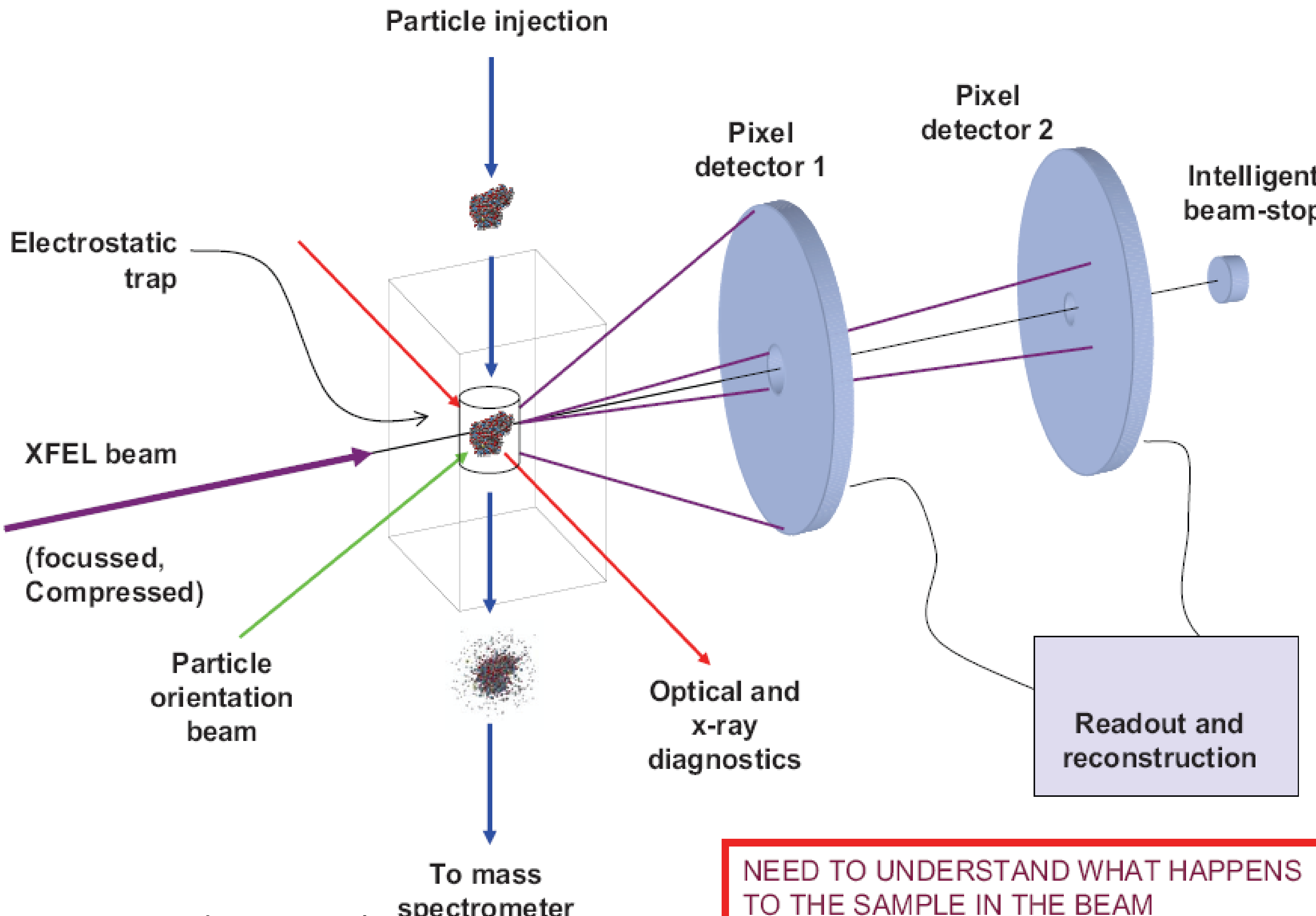
Concept: Capture an image with a short and intense X-ray pulse, before the sample has time to respond (explode)



3D reconstruction possible from many views

courtecy: Hajdu, Uppsala

Interaction chamber and detector arrangement



NEED TO UNDERSTAND WHAT HAPPENS TO THE SAMPLE IN THE BEAM

courtecy: Hajdu, Uppsala

Fundamentals of X-ray scattering

Brief history

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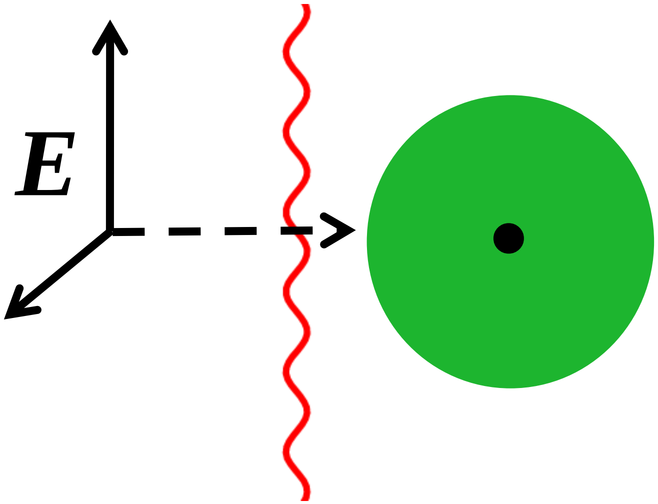
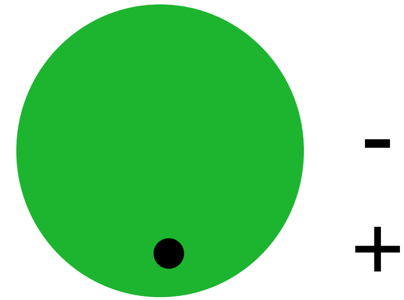
Darwin-breadth (qualitatively)

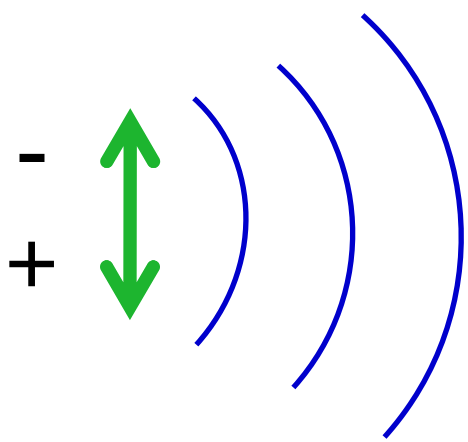
Monochromators (briefly)

Mechanism of X-ray scattering





the atom is polarized



the polarized dipole ***radiates***

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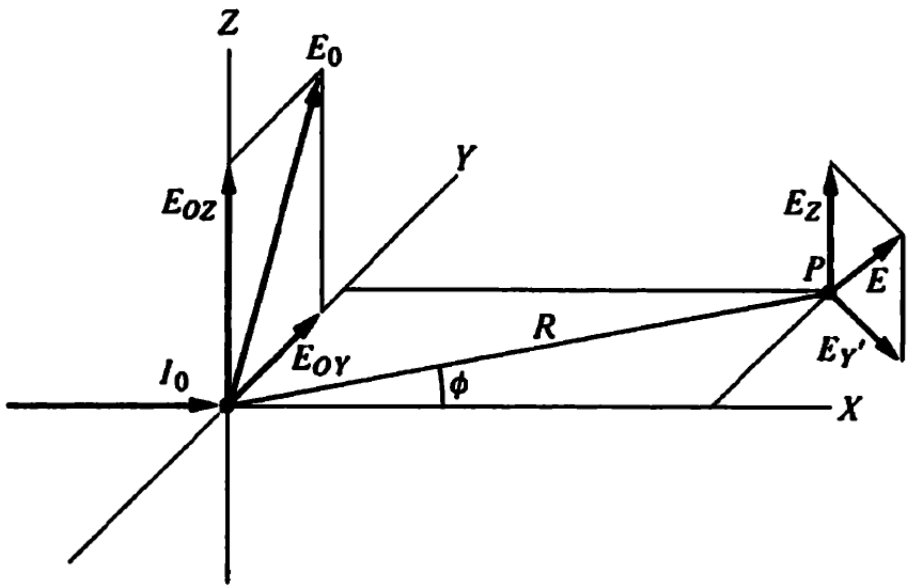
scattering of X-rays by an electron



$$\epsilon_{0Y'} = E_{0Y'} \sin 2\pi\nu t, \qquad \epsilon_{0Z} = E_{0Z} \sin 2\pi\nu t$$

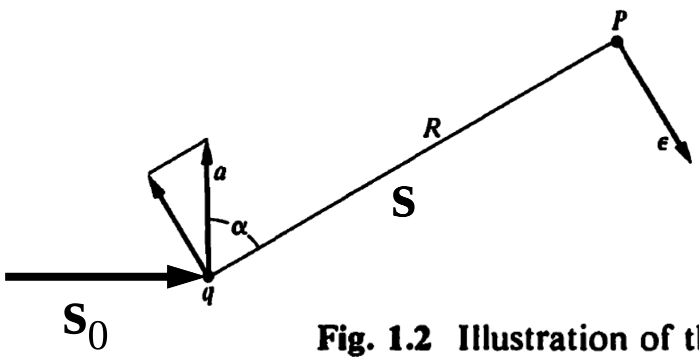


Fig. 1.2 Illustration of the electric field ϵ, produced by a charge q with acceleration a, according to classical electromagnetic theory.

the electric field, ε, in cgs units:

$$\epsilon = \frac{qa \sin \alpha}{c^2 R}$$

Warren, X-ray diffraction

scattering of X-rays by an electron

the Y' component of the electric field at P:

$$\epsilon_{Y'} = \frac{e^2 E_{0Y'}}{mc^2 R} \sin 2\pi\nu t \cos\phi$$

the amplitude is:

$$E_{0Y'} = \frac{e^2 E_{0Y'}}{mc^2 R} \cos\phi$$

the $\boldsymbol{E_{0Z}}$ amplitude (for the $\boldsymbol{E_Z}$ $\phi=90^o$) :

$$E_Z = \frac{e^2 E_{0Z}}{mc^2 R}$$

scattering of X-rays by an electron

the observed intensity at P:

$$E^2 = E_Z^2 + E_{Y'}^2 = \frac{e^4}{m^2c^4R^2}(E_{0Z}^2 + E_{0Y'}^2 \cos^2\phi)$$

assuming that the incoming beam is randomly polarized:

$$\langle E_{0Y'}^2 \rangle + \langle E_{0Z}^2 \rangle = \langle E_0^2 \rangle \quad \text{and} \quad \langle E_{0Y'}^2 \rangle = \langle E_{0Z}^2 \rangle = \tfrac{1}{2}\langle E_0^2 \rangle$$

finally:

$$\langle E^2 \rangle = \langle E_0^2 \rangle \frac{e^4}{m^2c^4R^2}\left(\frac{1+\cos^2\phi}{2}\right)$$

polarization factor
for an unpolarized
incoming beam

scattering of X-rays by an electron

the numerical factor in the scattered intensity:

$$\frac{e^4}{m^2c^4} = 7.94 \times 10^{-26}\ \text{cm}^2$$

the number of electrons in the volume illuminated by the incoming beam in a usual specimen:

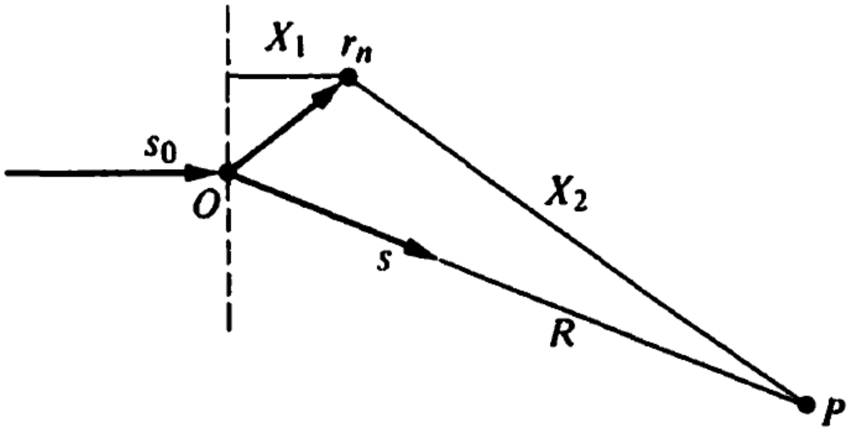
$$\sim 10^{22}$$

therefore, the scattered intensity is approximately of-the-order of:

$$I_{scattered} \sim I_0 \times 10^{-4}$$

Warren, X-ray diffraction

scattering of X-rays by an atom



$\boldsymbol{r}_n$ is the position of the n-th electron in the atom

the amplitude scattered by the n-th electron at P:

$$\epsilon_n = \frac{E_0 e^2}{mc^2 X_2} \cos\left[2\pi\nu t - \frac{2\pi}{\lambda}(X_1 + X_2)\right]$$

$\boldsymbol{X}_1 << \boldsymbol{X}_2$

it can be shown that:

$$X_1 + X_2 \rightarrow \mathbf{r}_n \cdot \mathbf{s}_0 + R - \mathbf{r}_n \cdot \mathbf{s} = R - (\mathbf{s} - \mathbf{s}_0) \cdot \mathbf{r}_n$$

Warren, X-ray diffraction

scattering of X-rays by an atom

turning to complex exponentials and summing over all electrons:

$$\epsilon = \frac{E_0 e^2}{mc^2 R} e^{2\pi i[\nu t - (R/\lambda)]} \sum_n e^{(2\pi i/\lambda)(\mathbf{s}-\mathbf{s}_0)\cdot\mathbf{r}_n}$$

scattering of X-rays by a smeared-out electron

$$\epsilon_e = \frac{E_0 e^2}{mc^2 R} e^{2\pi i[\nu t - (R/\lambda)]} \int e^{(2\pi i/\lambda)(\mathbf{s}-\mathbf{s}_0)\cdot\mathbf{r}} \rho \, dV.$$

electron scattering factor, f_e

ρ is the average charge-density distribution of the electron

f_e is the amplitude scattered by an electron in 1-electron-scattering-units

Warren, X-ray diffraction

scattering of X-rays by a smeared-out electron

taking into account the real charge-density distribution: $\rho(\boldsymbol{r})$

$$f_e = \int_0^\infty 4\pi r^2 \rho(r) \frac{\sin kr}{kr} dr$$

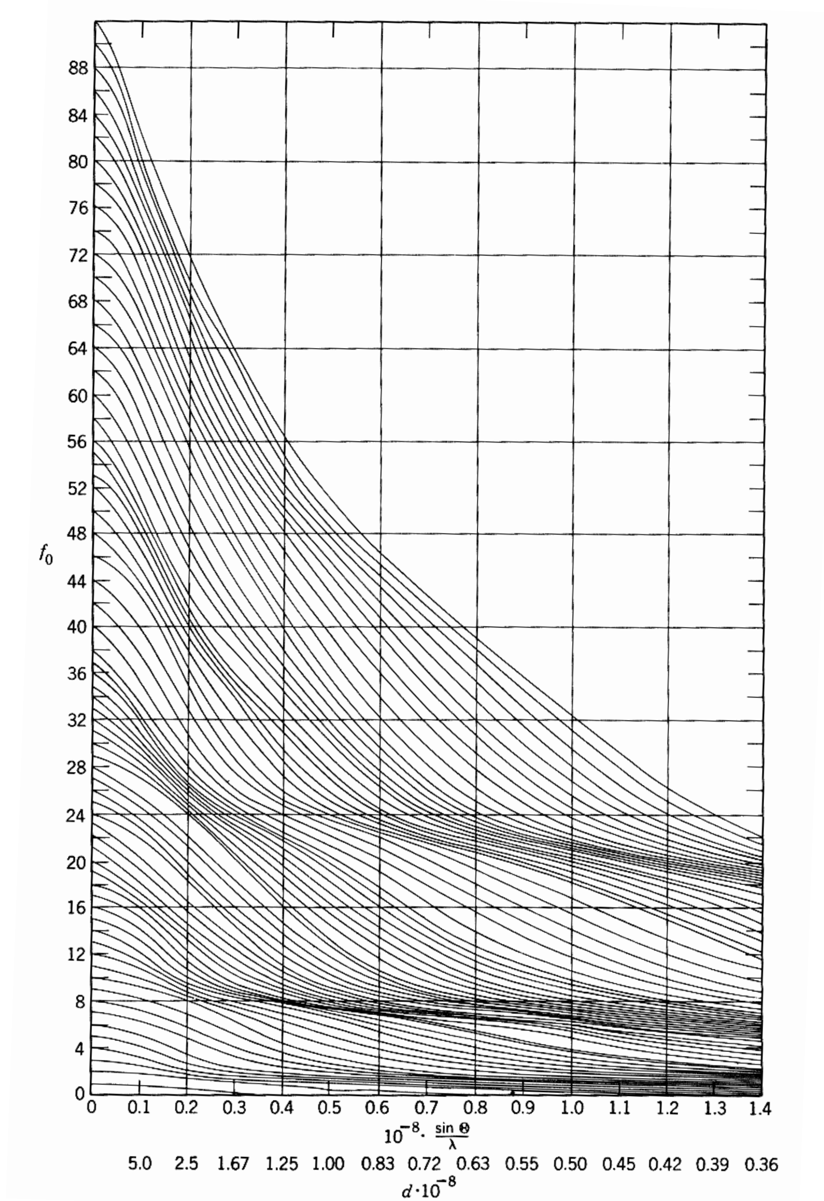
scattering of X-rays by an atom

the atomic scattering-factor:

$$f = \sum_n f_{en} = \sum_n \int_0^\infty 4\pi r^2 \rho_n(r) \frac{\sin kr}{kr} dr$$

f is measured in units of
scattering by a single electron

atomic scattering factors of X-rays



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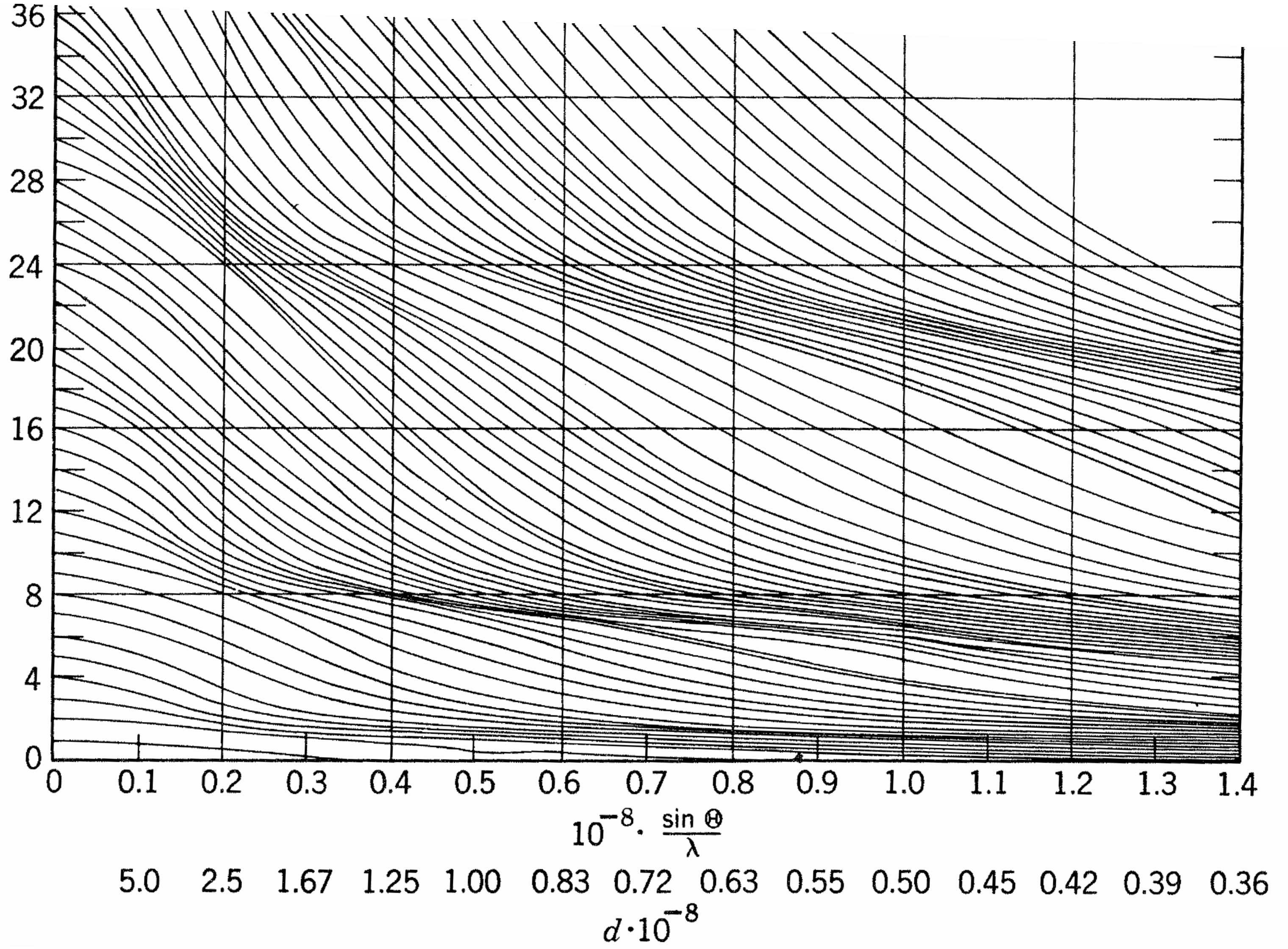
Klug & Alexander, X-ray diffraction

atomic scattering factors of X-rays



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Klug & Alexander, X-ray diffraction

atomic scattering factors of X-rays

$$f = \sum_n f_{en} = \sum_n \int_0^\infty 4\pi r^2 \rho_n(r) \frac{\sin kr}{kr} dr.$$

at k=0, where $k=4\pi sin\theta/\lambda$, $\sin kr/kr = 1$,
i.e. in the forward scattering case, or at small values of 2θ:

$$\sum_n \int_0^\infty 4\pi r^2 \rho_n(r)\, dr = Z$$

Warren, X-ray diffraction

comparison of scattering factors of X-rays and neutrons

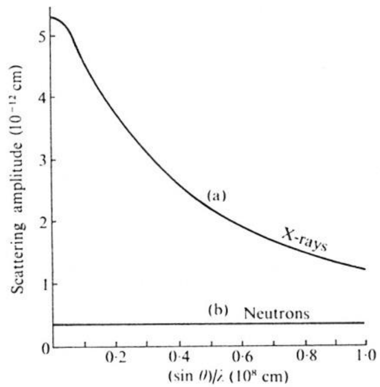

FIG. 16. X-ray and neutron scattering amplitudes for a potassium atom.

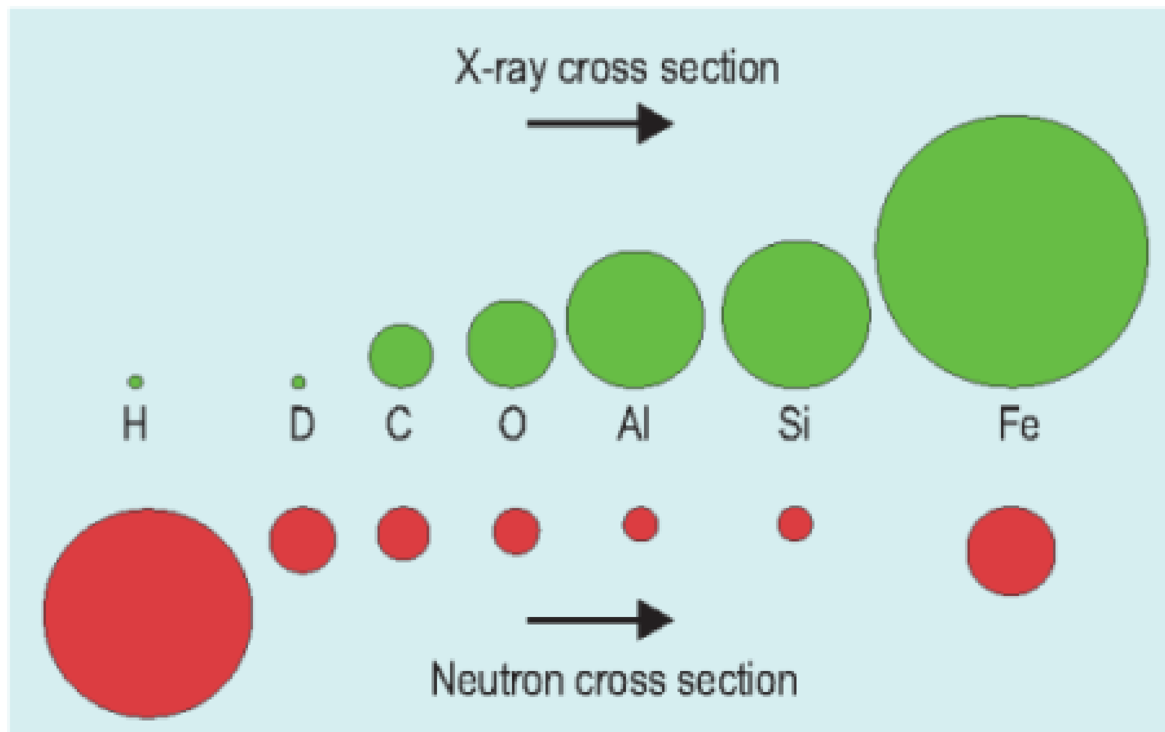

Fig. 2. Neutron and x-ray scattering cross-sections compared. Note that neutrons penetrate through Al much better than x rays do, yet are strongly scattered by hydrogen.

香港城市大學
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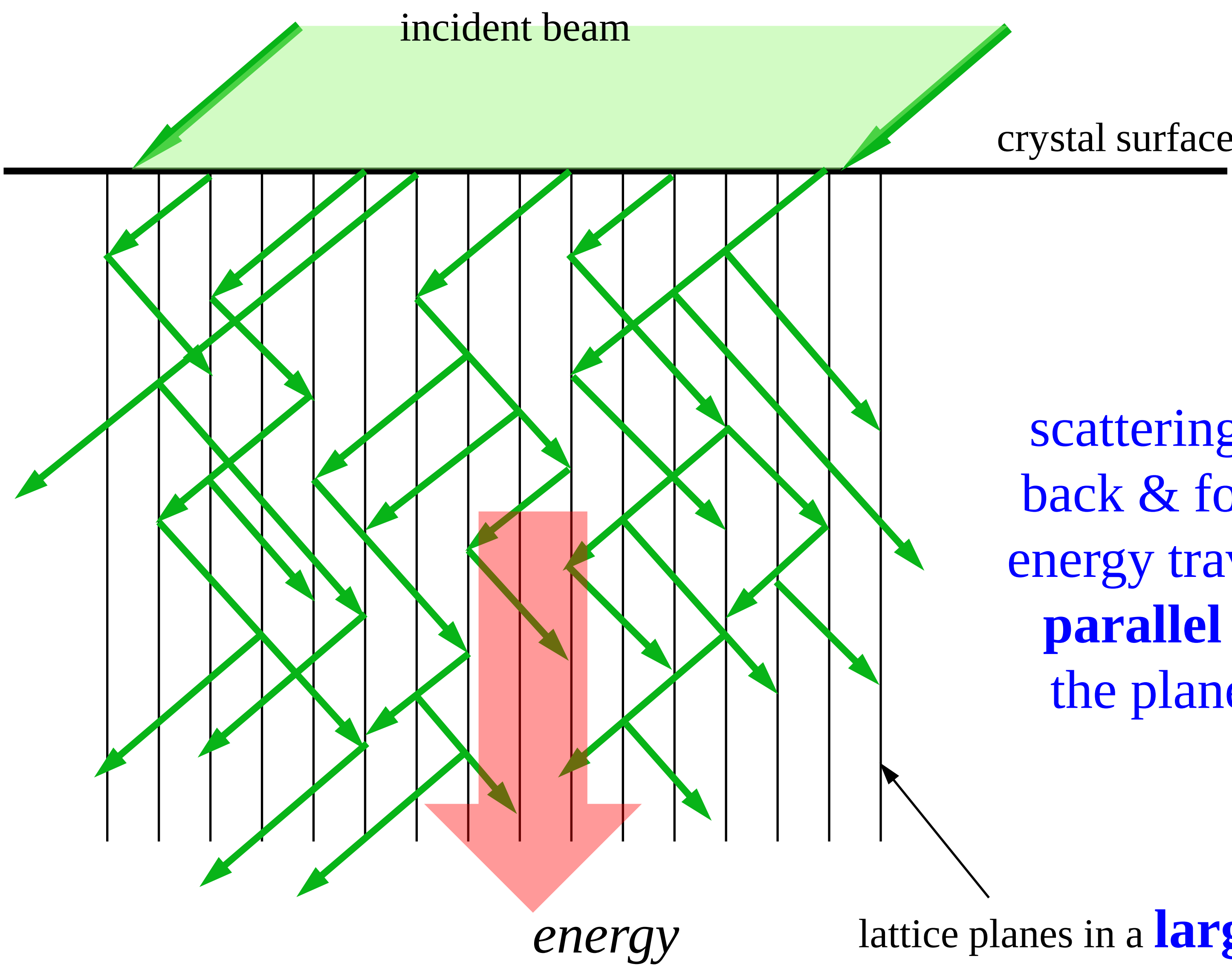
Fundamentals of X-ray scattering

Brief history
Laboratory X-ray sources,
Basic properties of X-rays,
X-ray spectra,
X-ray absorption edges,
Synchrotron X-ray sources,
Scattering mechanisms of X-rays by matter,
Atomic scattering factors for X-rays
Total X-ray reflection,
Darwin-breadth (qualitatively)
Monochromators (briefly)

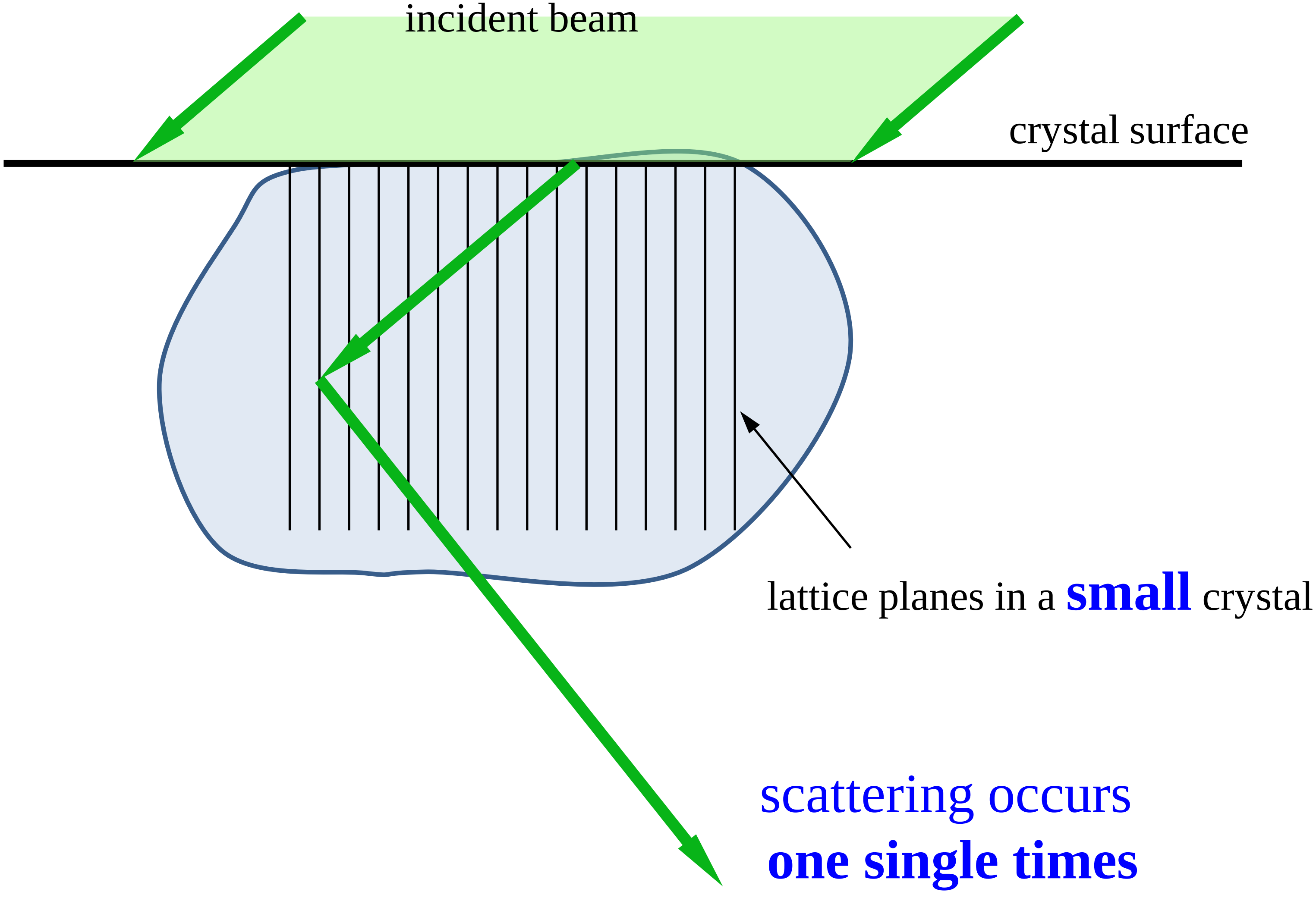
kinematical *vs.* dynamical scattering



scattering is back & forth energy travels **parallel** to the planes

lattice planes in a **large** crystal and **perfect**

kinematical *vs.* dynamical scattering



scattering occurs
one single times

kinematical *vs.* dynamical scattering

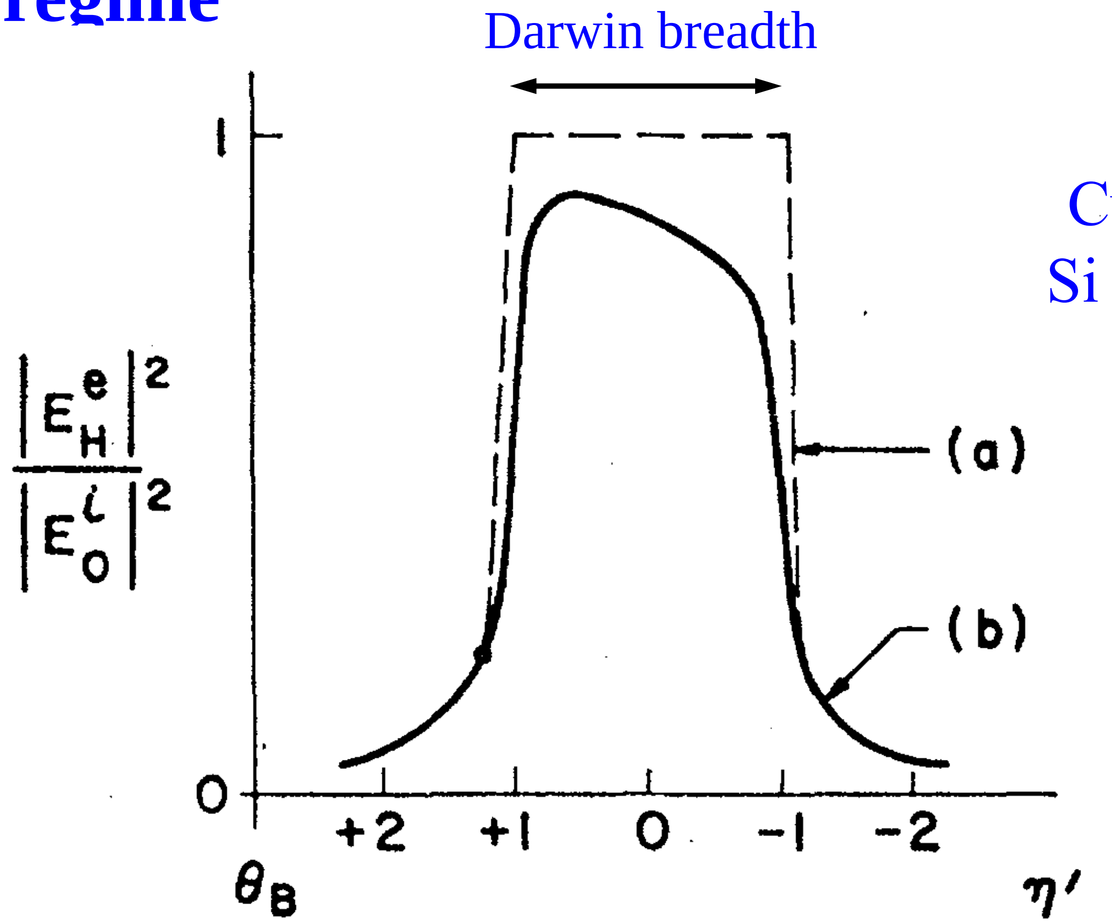
we want to deal with **small crystals**

where **scattering occurs one single times**:

this is: **kinematical scattering**

kinematical *vs.* dynamical scattering

monochromators are **large perfect** crystal
scattering occurs in the
dynamical regime



Cu (200): 19”
Si (220): 5.02”

http://www.chess.cornell.edu/oldchess/operatns/xrclcdwn.htm

Thank you