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Synchrotron Radiation - A Source for Spectroscopy and Structural Analysis in the Extreme Ultraviolet and Soft X-Ray Region

by

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SYNCHROTRON RADIATION - A SOURCE FOR SPECTROSCOPY AND STRUCTURAL ANALYSIS IN THE EXTREME ULTRAVIOLET AND SOFT X-RAY REGION

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For about ten years synchrotron radiation from high-energy synchrotrons and storage rings, besides being used to study beam behaviour in the machine, has also served as a radiation source in the extreme ultraviolet and soft X-ray region. The characteristics of the source (i.e. high intensity, continuous spectral distribution, polarization, good vacuum) make it superior to any other radiation source in the photon energy range between 10 eV and 10 keV.

Measurements using synchrotron radiation as an extreme ultraviolet and soft X-ray source are now being carried out in about 10 laboratories (mainly synchrotrons and one storage ring), but the number is increasing every year. Among the projects under construction is a storage ring which will only be constructed as a synchrotron radiation source.

A review is given on the experiments using synchrotron radiation and the requirements and possibilities of the different types of machines are outlined.

Invited paper given at the All Union Conference on High Energy Particle Accelerators, Oct. 2, 1972 in Moscow USSR, to be published in the Conference Proceedings.

When speaking about synchrotron radiation here in Moscow one has to be aware of treading on historical ground for. Several members of the university[1] developed the theory of synchrotron radiation and predicted among other details its influence on the maximum energy obtainable in cyclic electron accelerators and on the beam behaviour. The first beam diagnostic investigations have been performed at the synchrotron of the Lebedev Institute of the USSR Academy of Science.

The emphasis of my talk will lie on the use of electron synchrotrons and storage rings as sources of radiation in the extreme ultraviolet and soft X-ray range[2]. Here an interesting development took place: in the beginning spectroscopic work was mainly performed parasitically to the high energy experiments and it was the general opinion that the high costs for building and operating a synchrotron could not be justified by its use as a synchrotron radiation source alone. This opinion has now been changed: in Tokyo a storage ring is under construction only to be used as a vacuum ultraviolet source. Similar plans are being discussed intensively in the USSR and USA.

The realization of these plans will introduce a third generation of synchrotron radiation sources after the parasitically used synchrotrons (first generation) and storage rings (second generation).

Table I shows a compilation of the synchrotrons and storage rings of the first, second and third generation, where synchrotron radiation experiments have been performed or are under active preparation.

With the sources of the <u>first generation</u> mainly absorption, reflexion and photoelectron emission experiments have been performed on atomic and molecular gases and on solids[3].

Table I: Accelerators and storage rings used as synchrotron light sources

Projects	E(GeV)	R(m)	I(mA)	λ_c(Å)	Generation	Remarks
NBS (Washington)	.18	.83	1	800	I	
INS-SOR (Tokyo)	1.3	4.0	30	10	I	
Frascati	1.1	3.6		15	I	
DESY (Hamburg)	7.5	31.7	10-30	.3	I	
Wisconsin Storage Ring	.24	.54	10	220	III	
Glasgow	.33	1.25	0.1	195	I	
Bonn	2.3	7.65	30	3.5	I	
Moscow	0.68	2		35.6	I	
Erewan	6.0	24.65	22	0.64	I	
DNPL (Daresbury)	4.0	20.8	40	1.8	I	
CEA (Cambridge/Mass)	6.0	26.0	30	0.7	I or II	
INS-SOR (Tokyo) Storage Ring	0.3	1	100	200	III	planned for operation in 1974
ACO (Orsay) Storage Ring	.6	1.1	500	30	II	
SLAC (Stanford) Storage Ring	2.5 (3.5)	12.7	250	4.5	II	
DESY (Hamburg) Storage Ring	1.75 3.5	12.12	6000 200	12.7 1.58	II	planned for operation in 1973/74

Generation I = synchrotrons

Generation II = storage ring in parasitic use

Generation III = storage ring primarily used as a synchrotron light source

Figure 1 shows the spectral distribution[4] of the synchrotron radiation at DESY for different electron energies. The most interesting part is between 1 and 1000 Å, where all other conventional sources have intensities smaller by orders of magnitude. Only on the short wavelength end of this region have X-ray bremsstrahlungs sources of considerable intensities been developed by a group at the Leningrad University (Dr. T.M. Zimkina, Dr. V.A. Fomichev and collaborators) for spectroscopic (mainly absorption) studies.

Influenced by the working conditions in high energy laboratories the synchrotron radiation experiments are mostly performed by collaboration between different laboratories: at DESY 25 scientists from different german universities are working together in a laboratory whose interior is shown in Fig. 2 [5].

In the photon energy range under consideration (10 to 10,000 eV) electrons from different inner shells of the atoms can be excited. Figure 3 shows as a typical example the absorption spectrum of gaseous and solid Kr[6]. At 8 eV the onset of excitation from the 4p valence electron shell can be observed; near 90 eV evidence of the excitation of the 3d electrons can be seen. The features in the continuum absorption region are now well understood in terms of atomic theories which include many-body correlation effects.

The agreement of theory and experiment is not so good in the fine structure region near the onset of 3d-electron transitions. Figure 4 shows the experimental curve together with a theoretical density of state curve by Rössler[7]. Here the theoretical solid state approach may be improved by also taking into account many-body effects.

The basic question is: to what extent are band structure and density of states calculations, based on the whole solid and its periodic crystalline structure, good for describing inner shell transitions, which are more localized , since the initial state wavefunction is confined to the neighbourhood of the nucleus.

A deeper insight may be obtained from photoelectron energy distribution experiments, from luminescence, fluorescence or from molecular fragmentation studies. Here the intensity from sources of the first generation sets limits; higher intensities, as obtainable from the storage rings, at least of the second generation, are required. Besides the higher beam current another attraction of storage rings is the high stability which allows the application of more refined experimental techniques as e.g. moldulation spectroscopy.

In the shorter wavelength region other experiments such as Comptcn scattering or diffraction experiments come into discussion. At DESY first experiments on X-ray diffraction on specimens of interest in molecular biology[8] have been performed by a group from the Max-Planck-Institut für Medizinische Forschung in Heidelberg. It has been shown that exposure times in diffraction experiments can been shortened by a factor of 30 as compared to the use of normal X-ray tubes (Cu K_{α} radiation at 1.5 keV). This success led to the construction of a second laboratory at the synchrotron to be used mainly for biomolecular studies. Furthermore, two laboratories for spectroscopic and biomolecular investigations will be available at the storage ring DORIS now under construction and to come into operation in 1973/74.

The increasing interest in synchrotron radiation experiments finally led to the consideration of machines of the third generation, storage rings which are constructed exclusively as synchrotron radiation sources. These machines will have different advantages not met by the parasitic use of machines of the first and second generation:

a) Only one beam is necessary which can be optimized without regarding a second colliding beam. Thus beam - beam interaction and their mutually induced instabilities do not play any role.

b) Current and energy can be controlled according to the needs of synchrotron radiation users.

c) By introducing high field magnetic assemblies (wigglers) in straight sections the intensity can be increased at different points of the circumference.

d) The beam size can be minimized at the tangential points where the radiation is taken off. This is of special importance for experiments where high energy resolution is required.

Machines of the third generation must not necessarily be those, which were primarily constructed as synchrotron radiation sources as the Tokyo storage ring. They can also be machines, which for different reasons, are no longer used by high energy physicists. The first example of this category was the Storage Ring of the Physical Sciences Laboratory in Stoughton, Wisconsin and others may follow in the future.

References:

1. A.A. Sokolov and I.M. Ternov, Synchrotron Radiation (Pergamon Press, 1968) and references therein

2. R.P. Godwin, in Springer Tracts in Modern Physics, ed. G. Höhler (Springer Verlag, Berlin 1969) Vol. 51, p. 1

3. R. Haensel and B. Sonntag, in Computational Physics, ed. F. Herman, N.W. Dalton and Th.R. Koehler, (Plenum Press, New York 1972) p. 43

4. R. Haensel and C. Kunz, Z.Angew. Phys. 23, 276 (1967)

5. C. Kunz, in Band Structure Spectroscopy of Metals and Alloys, ed. D.J. Fabian and L.M. Watson (Academic Press, London 1973) p. 503

6. P. Schreiber, thesis, University of Hamburg 1970 (unpublished) Internal report DESY F41-70/6

7. U. Rössler, phys.stat.sol. (b) 45, 483 (1971)

8. G. Rosenbaum, K.C. Holmes and J. Witz, Nature 230, 434 (1971)

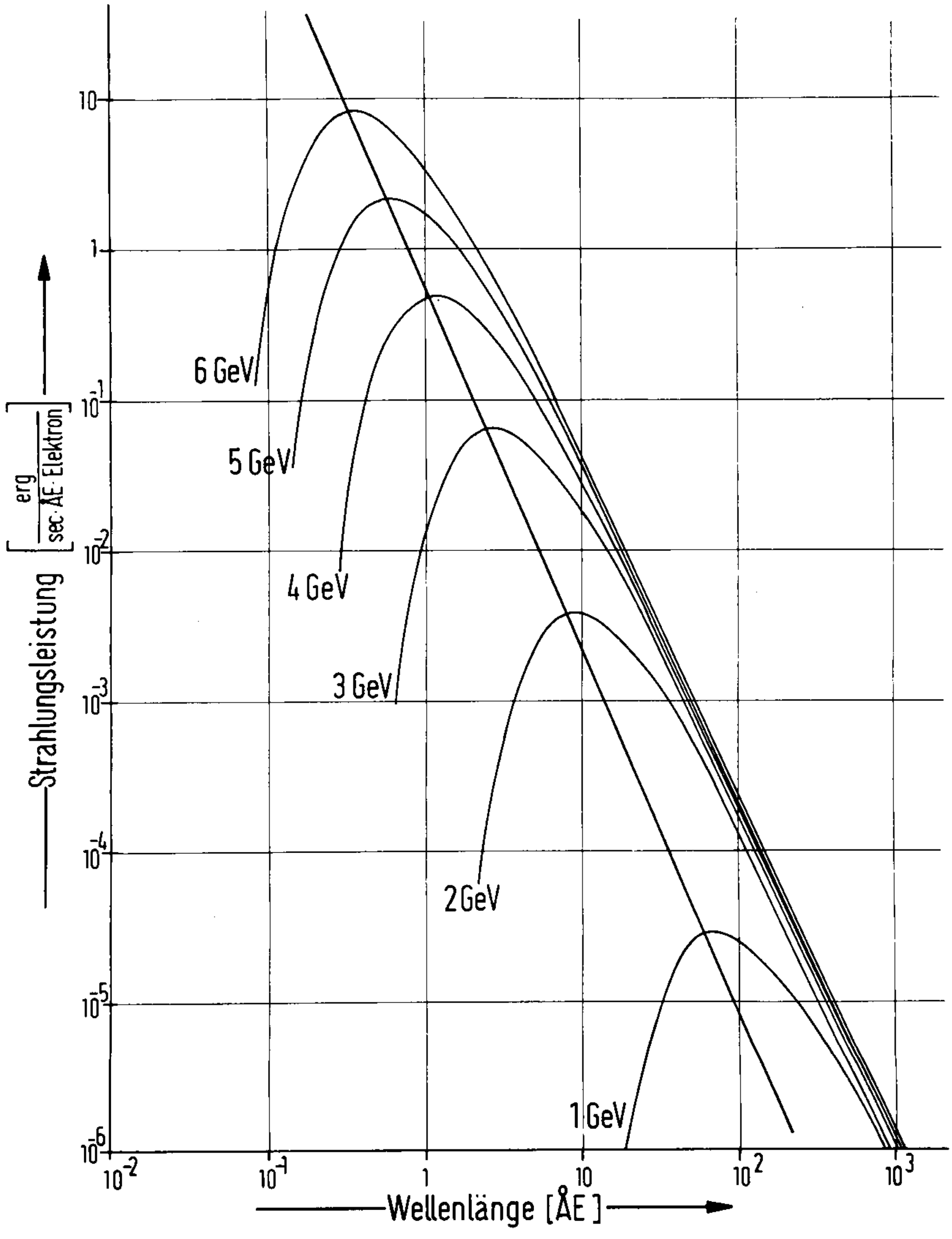
Figure Captions:

Fig. 1 Spectral distribution of synchrotron radiation emitted by DESY (R = 31.87 m) at different electron energies

Fig. 2 Cross-section of the synchrotron radiation laboratory at DESY[5]

Fig. 3 Optical absorption of gaseous and solid Kr in the energy range 9 to 1000 eV[6]

Fig. 4 Fine structure of the 3d-absorption of solid Kr in comparison to the density of states curve[7]



10
1
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-2}
10^{-1}
1
10
10^{2}
10^{3}
6 GeV
5 GeV
4 GeV
3 GeV
2GeV
1 GeV
Strahlungsleistung $\left[\frac{\text{erg}}{\text{sec} \cdot \text{ÅE} \cdot \text{Elektron}}\right]$
Wellenlänge [ÅE]

Figure 1

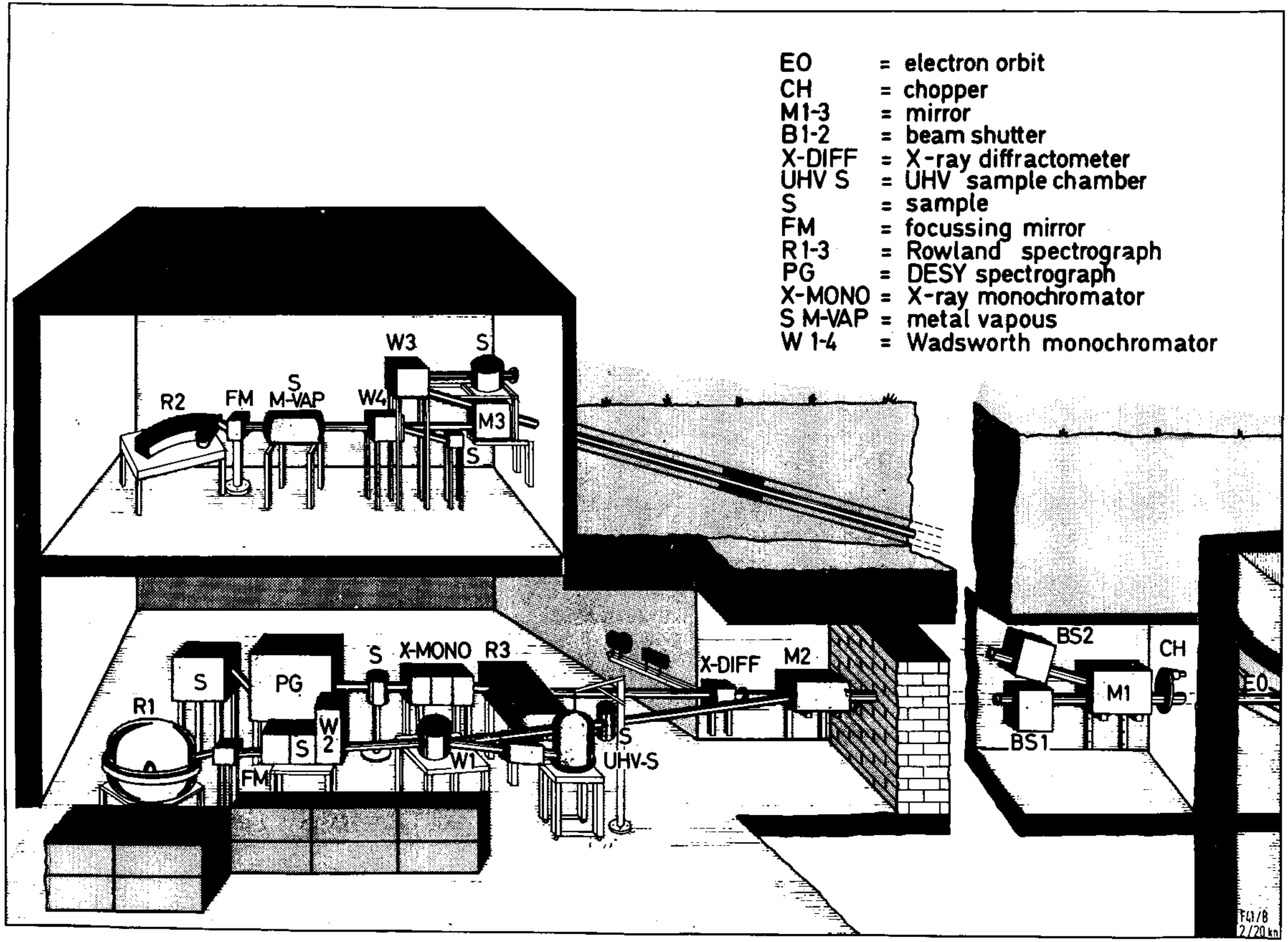

EO = electron orbit
CH = chopper
M1-3 = mirror
B1-2 = beam shutter
X-DIFF = X-ray diffractometer
UHV S = UHV sample chamber
S = sample
FM = focussing mirror
R1-3 = Rowland spectrograph
PG = DESY spectrograph
X-MONO = X-ray monochromator
S M-VAP = metal vapous
W 1-4 = Wadsworth monochromator
W3
S
R2
FM
S M-VAP
W4
M3
S
S
PG
S
X-MONO
R3
X-DIFF
M2
BS2
CH
M1
EO
R1
S
W 2
W1
S
UHV-S
FM
BS1

Figure 2

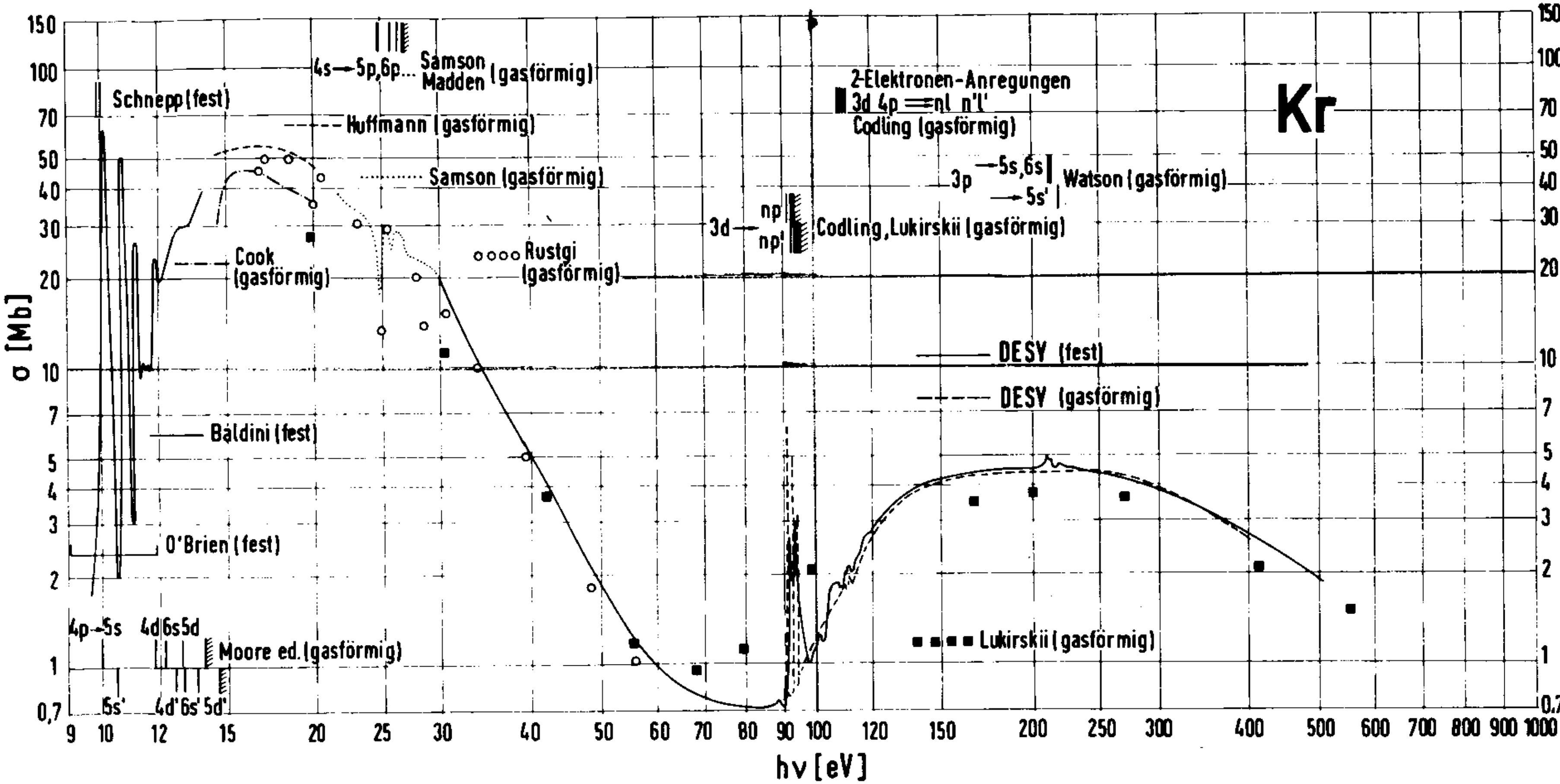
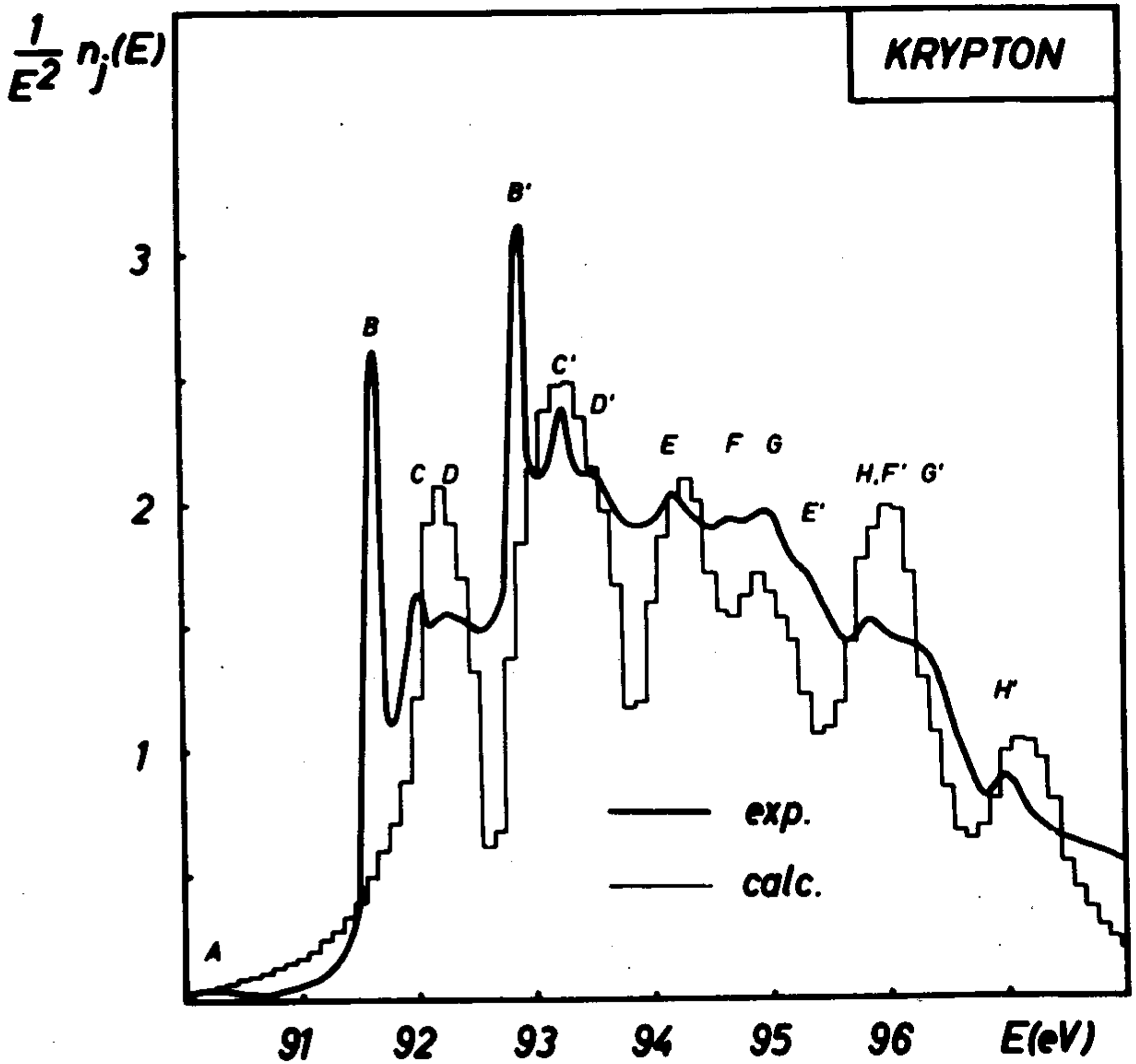

Kr
Schnepp (fest)
4s → 5p,6p...
Samson Madden (gasförmig)
Huffmann (gasförmig)
Samson (gasförmig)
Cook (gasförmig)
Rustgi (gasförmig)
Baldini (fest)
O'Brien (fest)
Moore ed. (gasförmig)
4p→5s
4d 6s 5d
6s'
4d' 6s' 5d'
2-Elektronen-Anregungen
3d 4p ⇉ nl n'l'
Codling (gasförmig)
3p → 5s, 6s
→ 5s'
Watson (gasförmig)
3d → np
np'
Codling, Lukirskii (gasförmig)
DESY (fest)
DESY (gasförmig)
Lukirskii (gasförmig)
σ [Mb]
hν [eV]

Figure 3



$\frac{1}{E^2} n_j(E)$
KRYPTON
B'
3
B
C'
D'
C D
E F G
H,F' G'
2
E'
H'
1
exp.
calc.
A
91
92
93
94
95
96
E(eV)

Figure 4