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MASTER

WORKSHOP ON ATOMIC PHYSICS AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

HELD AT
BROOKHAVEN NATIONAL LABORATORY
SEPTEMBER 15-17, 1980

JANUARY 1981
INFORMAL REPORT

BROOKHAVEN NATIONAL LABORATORY
ASSOCIATED UNIVERSITIES, INC.
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Held at

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DISCLAIMER

K. W. Jones, B. M. Johnson, and D. C. Gregory

Editors

January 1981

INFORMAL REPORT

B R O O K H A V E N N A T I O N A L L A B O R A T O R Y

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PREFACE

A workshop on "Atomic Physics at the National Synchrotron Light Source" (NSLS) was held at Brookhaven National Laboratory on September 15-17, 1980, with an attendance of approximately 45 scientists from several disciplines. The purpose of the meeting was to acquaint the atomic physics community with the range of experimental capabilities that will be open to them when the NSLS goes into operation and to endeavor to stimulate thinking about the types of atomic physics experiments that could be carried out at this new facility. We hope that these proceedings will help to convey the enthusiasm and interest which were expressed during the workshop and will serve to stimulate further consideration of the topic.

T. H. Kruse (Rutgers) and V. O. Kostroun (Cornell) were outside members of the organizing committee. We are especially indebted to Bernd Crasemann for coming so far to open and close our proceedings, to Arie Van Steenbergen and the staff of the NSLS for their cooperation and informative contributions, Jules Godel and George Hummer for the tour of the NSLS facility, and to all the speakers for their amazing promptness in supplying manuscripts.

We particularly extend our thanks to Lore Barbier, the workshop secretary, for her very efficient organization of all the tedious details of the workshop and preparation of the proceedings.

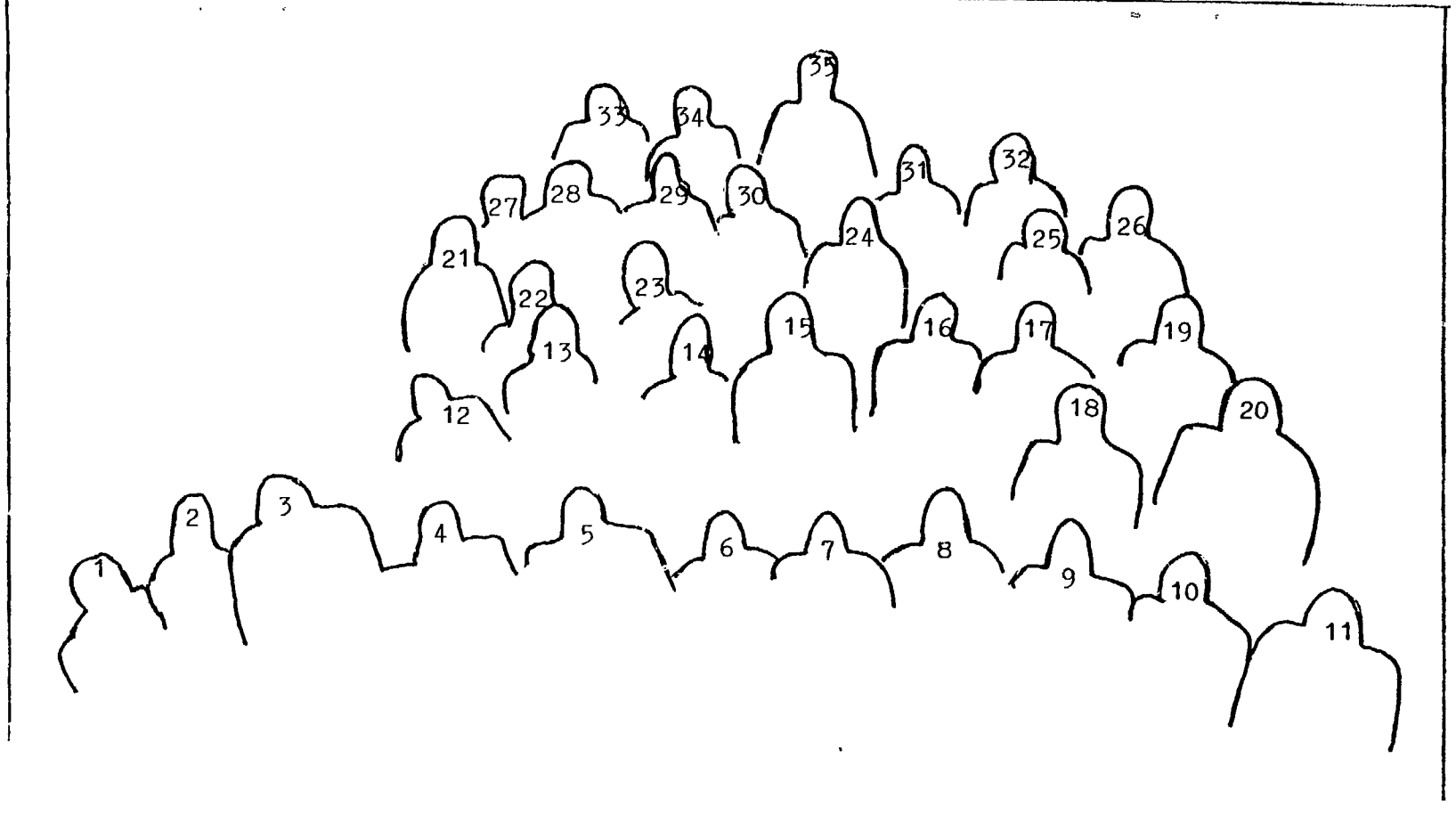
We also gratefully acknowledge the interest and support for the workshop received from Dr. J. V. Martinez, Fundamental Interactions Branch, Division of Chemical Sciences, Office of Basic Energy Sciences of the Department of Energy.

K. W. Jones, B. M. Johnson, D. C. Gregory
The Editors

January 1981

Workshop on Atomic Physics at the National Synchrotron Light Source

Brookhaven National Laboratory - September 15-17, 1980



1 - A. Z. Schwarzschild
2 - P. R. Woodruff
3 - D. A. Church
4 - H. Kelly
5 - J. A. R. Samson
6 - R. P. Chaturvedi
7 - K. W. Jones
8 - J. P. Delvaille
9 - J. D. Larson
10 - Y-K. Kim
11 - C. M. Brown
12 - W. W. Smith
13 - B. Crasemann
14 - M. G. White
15 - T. A. Carlson
16 - P. Koch
17 - L. Armstrong
18 - S. T. Manson
19 - B. M. Johnson
20 - G. Basbas
21 - J. Davenport
22 - J. W. Cooper
23 - R. Klaffky
24 - W. Brandt
25 - T. H. Kruse
26 - P. M. Griffin
27 - R. M. Sinclair
28 - W. Savin
29 - M. Blume
30 - V. W. Hughes
31 - J. R. Grover
32 - S. M. Shafroth
33 - D. C. Gregory
34 - V. O. Kostroun
35 - R. E. Watson

TABLE OF CONTENTS

Program ix

List of Participants. xi

Atomic Physics Research with Synchrotron Radiation
B. Crasemann. 1

Photoionization of Excited States, Ions and Open-Shell Atoms: Innovative Synchrotron Experiments
S. T. Manson. 13

Atomic Structure and Electron Correlations
H. P. Kelly 19

Transition Probabilities for Atoms
Y-K. Kim. 33

Photoelectron Spectroscopy and Photoionization Experiments on Atoms and Free Molecules
T. A. Carlson 43

Possible Applications of Synchrotron Radiation to X-Ray Astrophysics
J. P. Delvaille 49

NSLS Machine Parameters and Hardware. 53

An Apparatus for Gas Phase Studies at $\lambda \geq 300$ Å
J. R. Grover and M. G. White. 71

Multiply Charged Ion Sources for Photon-Ion Crossed Beam Experiments
V. O. Kostroun. 79

Constraints on Ion Beam Handling for Intersecting Beam Experiments
T. H. Kruse 95

Low Energy Ion Storage Devices
D. A. Church. 101

Photon Detection in the VUV
J. A. R. Samson 117

Electron Spectrometers
P. R. Woodruff. 129

BNL Plans for Atomic Physics at the NSLS
K. W. Jones 137

Possible Future Experiments in Atomic Physics Utilizing Synchrotron Radiation
J. W. Cooper. 145

Applications of Atomic and Molecular Synchrotron Experiments to Condensed Matter Physics
J. W. Davenport 153

Use of Synchrotron Radiation for Development of UV and X-Ray Detectors for Particle and Nuclear Physics
D. C. Lu and V. W. Hughes 157

Polarization of Photoelectrons Produced from Atoms by Synchrotron Radiation
V. W. Hughes, D. C. Lu, and K. N. Huang 159

Negative Ions, Production of Slow High-q Ions, Collisions with Inner-Shell Excited Targets Using Synchrotron Radiation
W. W. Smith 163

General Discussion Session
B. Crasemann, Chairman. 169

Working Group Summary - Areas for Study at NSLS
S. T. Manson, Leader. 191

Working Group Summary - Hardware
T. H. Kruse, Leader 195

Concluding Remarks
B. Crasemann. 199

FINAL PROGRAM

WORKSHOP ON ATOMIC PHYSICS AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

Berkner Hall, Room B

Monday, September 15, 1980

Chairman:	M. BLUME - *BNL*
9:00	Introduction
9:15	B. CRASEMANN - *University of Oregon* Atomic Physics Research with Synchrotron Radiation (30 min.)
10:00	S. T. MANSON - *Georgia State University* Photoionization of Excited States, Ions, and Open-Shell Atoms: Innovative Synchrotron Experiments (30 min.)
10:45	Coffee
11:00	H. P. KELLY - *University of Virginia* Atomic Structure and Electron Correlations (30 min.)
11:45	Y. K. KIM - *Argonne National Laboratory* Transition Probabilities of Atomic States (30 min.)
12:30	Lunch
Chairman:	W. W. SMITH - *University of Connecticut*
2:00	P. M. KOCH - *Yale University* Highly Excited Atoms (30 min.)
2:45	T. A. CARLSON - *Oak Ridge National Laboratory* Photoelectron Spectroscopy and Photoionization Experiments on Atoms and Free Molecules (30 min.)
3:30	Coffee
3:45	J. P. DELVAILLE - *Smithsonian Center for Astrophysics* Possible Applications of Synchrotron Radiation to Astrophysics (30 min.
4:30	A. VAN STEENBERGEN - *BNL* The National Synchrotron Light Source (15 min.)
4:45	Tour of the NSLS Facility (30 min.)
6:00	Complimentary Cocktails - Berkner Hall
7:00	Banquet - Berkner Hall

Tuesday, September 16, 1980

Chairman: B. M. JOHNSON - *BNL*

9:00 W. BRANDT - *New York University*
Discussion Period

10:00 J. B. HASTINGS - *BNL*
Monochromators and Beam Lines for the NSLS X-Ray Ring (15 min.)

M. R. HOWELLS - *BNL*
Monochromators and Beam Lines for the NSLS VUV Ring (15 min.)

10:45 Coffee

11:00 J. R. GROVER - *BNL*
Gas Phase Spectroscopy in the VUV (15 min.)

11:30 V. O. KOSTROUN - *Cornell University*
Sources of Highly Charged Ions (15 min.)

T. H. KRUSE - *Rutgers University*
Constraints on Ion Beam Handling (15 min.)

K. H. PURSER - *General Ionex*
Ion Beam Handling Techniques (15 min.)

12:45 Lunch

Chairman: V. O. KOSTROUN - *Cornell University*

2:00 D. A. CHURCH - *Cyclotron Institute, Texas A & M University*
Low Energy Ion Storage Devices (30 min.)

2:45 J. A. R. SAMSON - *University of Nebraska*
Photon Detection in the VUV (20 min.)

3:15 Coffee

3:30 P. R. WOODRUFF - *University of Wisconsin Synchrotron*
Electron Spectrometers (20 min.)

4:00 V. RADEKA - *BNL*
Position Sensitive X-Ray Detectors (20 min.)

4:30 K. W. JONES - *BNL*
Plans for the Atomic Physics Beam Line at the NSLS (15 min.)

6:00 Cars leave Berkner Hall for dinner trip to Port Jefferson

Wednesday, September 17, 1980

9:00 D. C. GREGORY - *BNL*
Guidelines for Preparation of Workshop Report (15 min.)

9:15 B. CRASEMANN - *University of Oregon*
General Discussion Period

10:00 Split into Working Groups

Physics Group - Room B	Hardware Group - Room C
Leader - S. T. MANSON	Leader - T. H. KRUSE

11:00 Coffee

11:15 Presentation of Working-Group Summaries

12:00 B. CRASEMANN - *University of Oregon*
Concluding Remarks

WORKSHOP ON ATOMIC PHYSICS AT THE NATIONAL SYNCHROTRON LIGHT SOURCE

Brookhaven National Laboratory, September 15-17, 1980

Participants

L. Armstrong	Johns Hopkins University
G. Basbas	Physical Review Letters
M. Blume	Brookhaven National
W. Brandt	New York University
C. M. Brown	Naval Research Laboratory
T. A. Carlson	Oak Ridge National Laboratory
R. P. Chaturvedi	State University of New York - Cortland
D. A. Church	Texas A & M University
J. W. Cooper	National Bureau of Standards
B. Crasemann	University of Oregon
J. Davenport	Brookhaven National Laboratory
J. P. Delvaille	Smithsonian Center for Astrophysics
D. C. Gregory	Brookhaven National Laboratory
P. M. Griffin	Oak Ridge National Laboratory
J. R. Grover	Brookhaven National Laboratory
J. B. Hastings	Brookhaven National Laboratory
M. R. Howells	Brookhaven National Laboratory
V. W. Hughes	Yale University
B. M. Johnson	Brookhaven National Laboratory
K. W. Jones	Brookhaven National Laboratory
H. Kelly	University of Virginia
Y-K. Kim	Argonne National Laboratory
R. Klaffky	Brookhaven National Laboratory
P. Koch	Yale University
V. O. Kostroun	Cornell University
T. H. Kruse	Rutgers University
J. D. Larson	
D. Lu	Yale University
R. P. Madden	National Bureau of Standards
S. T. Manson	Georgia State University
K. H. Purser	General Ionex Corporation
V. Radeka	Brookhaven National Laboratory
J. A. R. Samson	University of Nebraska
W. Savin	New Jersey Institute of Technology
A. Z. Schwarzschild	Brookhaven National Laboratory
S. M. Shafroth	University of North Carolina
R. M. Sinclair	National Science Foundation
W. W. Smith	University of Connecticut
R. M. Sternheimer	Brookhaven National Laboratory
A. Van Steenbergen	Brookhaven National Laboratory
R. E. Watson	Brookhaven National Laboratory
M. G. White	Brookhaven National Laboratory
G. P. Williams	Brookhaven National Laboratory
P. R. Woodruff	University of Wisconsin Synchrotron

ATOMIC PHYSICS RESEARCH WITH SYNCHROTRON RADIATION*

Bernd Crasemann

Department of Physics, University of Oregon
Eugene, Oregon 97403

1. Introduction

The use of synchrotron radiation for experiments in atomic physics is quite new: It has been less than twenty years since Madden and Codling performed their classic experiment on the NBS 180-MeV electron synchrotron, in which they made the first observation of two-electron excitations in He leading to autoionizing levels.[1,2] In the brief intervening period, and particularly with the advent of major dedicated synchrotron-radiation sources in the last few years, the potential of tunable $h\nu$ for the study of atomic and molecular structure and transitions has become widely recognized.[3-5] To be sure, not everyone is happy with synchrotron radiation. We read that the new LEP (Large Electron-Positron) colliding-beam accelerator being erected by CERN on the French-Swiss border, with a 30-km circumference, will have to draw 250 megawatts of electrical power from the French electricity grid when operating at 90 GeV, primarily to make up for radiation losses.[6] Fortunately, the word "losses" is hardly appropriate for the photons that will be spewing from electrons orbiting in the NSLS storage rings, and it is our exciting task at this workshop to speculate on the important research in atomic physics that this powerful new facility will make possible.

While investigations in atomic physics with synchrotron radiation have mushroomed since Madden and Codling's pioneering work, it is

interesting to note that the bulk of this work has been in the ultraviolet regime. In fact, François Wuilleumier, one of the foremost investigators in the field, when reviewing "Atomic Physics with Synchrotron Radiation" at the XIth International Conference on the Physics of Electronic and Atomic Collisions in Kyoto last year, made this simple statement at the end of his talk: "In the x-ray region, very little has been achieved so far, but photoelectron and Auger spectroscopies are already feasible."[7] And at the International Conference on X-Ray Processes and Inner-Shell Ionization held in Scotland only two weeks ago, I eagerly listened to C. Kunz's Keynote Paper entitled "Photoemission Investigation of Inner Shells with Synchrotron Radiation," only to find that this otherwise excellent review cut off well below 1 keV photon energy, and did not penetrate to shells more "inner" than 3d or 4f in the rare earths.[8] It is for this reason, as well as due to my long-standing concern with atomic inner-shell processes, that I am led to believe that the virgin territory, in which some of the major potential lies for atomic research with synchrotron radiation, comprises the hard-x-ray regime from a few keV to several tens of keV photon energy. In the area of deep inelastic photon interactions, (truly) inner-shell photoelectron and Auger spectrometry, the investigation of threshold and resonance phenomena and of the dynamics of atomic relaxation --- here, I think, opportunities for some very important and fundamental work exist.

2. Research Opportunities

I will briefly summarize some particularly attractive applications of synchrotron radiation to research in high-energy atomic physics.

These lie in the areas of photoelectron spectrometry, photon scattering, x-ray absorption spectrometry, time-resolved measurements, and, very importantly, in the category of new applications yet to be devised.

2.1 Photoelectron Spectrometry with Synchrotron Radiation

Use of a tunable synchrotron radiation source permits the study of the features of a photoelectron spectrum as they vary with incident-photon energy. This subject has been expertly analyzed in a recent review by Manfred Krause;[9] Steve Manson and Tom Carlson will discuss the subject in more detail later in this Workshop. The main point is that a tunable x-ray source combined with photoelectron spectrometry makes it possible to probe the structure of atomic and molecular systems with high differentiation, and to look for many-electron effects in bound and continuum states, to trace multiple deexcitation pathways, and generally, to complement experimentally the recent advances in theory that include many-body and relativistic effects (Table I).

TABLE I. Photoelectron Spectrometry with Synchrotron Radiation.[a]

Partial Photoionization Cross Sections Angular Distribution of Photoelectrons	Contributions from Various Subshells Contributions from Multielectron Transitions Autoionization and Resonances
Energies of Photoelectrons and Auger Electrons	Correlation Satellites Molecular Dissociation Post-Collision Interaction Level and Line Widths

[a]See M. O. Krause, in Synchrotron Radiation Research, ed. by S. Doniach and H. Winick (Plenum, New York, 1980).

2.2 Photon Scattering

The intensity, tunability, and polarization of synchrotron radiation make it ideal for experiments on x-ray scattering, particularly on inelastic scattering. There are several reasons why work in this area is important.

Electron-electron Coulomb correlation.- The elastic-scattering form factor is the Fourier transform of the radial charge distribution. The total-scattering form factor, on the other hand, is the transform of the electron-electron distribution function. For this reason, the total x-ray differential cross section is exceedingly sensitive to correlation.[11] Figure 1 shows the measured x-ray scattering cross section of H_2, compared with a Hartree-Fock calculation and with cross sections computed by Bentley and Stewart[12] from a natural-orbital expansion of the Kolos-Roothaan correlated H_2 wave functions.

Electron momentum distributions.- These distributions can be derived from Compton profiles; there is an excellent book on the subject, by Brian Williams.[13]

Collective excitations.- Going beyond atomic physics proper, it is worth while to point out the superiority of x-ray scattering over electron beam techniques for the study of collective excitations in solids, where large momentum transfers are involved. The larger range of x rays and the reduced role of multiple scattering constitute important advantages. Hard x rays (30-50 keV) in particular are expected to be used for inelastic scattering experiments to investigate plasmons.[14]

2.3 Absorption Spectrometry

While x-ray absorption spectrometry constitutes one of the oldest uses of synchrotron radiation,[15] new sources have given it fresh impetus ---

in solid state and materials research through EXAFS, and in atomic physics in such applications as the precision determination of energy levels.[16] In Fig. 2 we see a high-resolution spectrum of the Kr K edge, and the theoretical model for the edge constructed by M. Breinig.[16] Comparison of energy-level intervals from this spectrum with optical data shows exceedingly good agreement, and the technique leads to level-energy determinations with a precision that can help establish many-body, relativistic and QED shifts.

2.4 Time-Resolved Spectroscopy

The pulse structure of synchrotron radiation lends itself to possibilitites that range from time-of-flight electron spectrometry[17] to a large variety of time-development measurements and coincidence experiments. The latter, in particular, can be used to further increase the selectivity of synchrotron-radiation studies of complex systems in which a large number of excitation and deexcitation channels exist. Initial work of this nature has been performed in the UV domain at DESY, ACO, and NBS, primarily in connection with molecular spectroscopy.[9] The power of time-of-flight analysis in resonance photoelectron spectroscopy has been demonstrated by Rosenberg et al.[18] in a beautiful experiment on autoionizing states of atomic Ba; the SPEAR pulse structure was used to obtain photoelectron spectra that were unaffected by fluctuations in synchrotron beam current and sample number density, with very high efficiency and excellent signal-to-noise ratios. The technique was shown to be capable of generating a whole new class of information about the electronic structure of autoionizing states. Yet, in the x-ray regime,

the time structure of synchrotron radiation is to date perhaps the least exploited feature of this source, and it holds great promise.

2.5 Resonance Spectroscopy and Threshold Excitation

Highly monochromatized, hard synchrotron radiation can be used in a particularly interesting way to study threshold excitation and resonance effects in inner shells of atoms. The x-ray resonant Raman effect, originally discovered by Sparks,[19] was investigated by Eisenberger et al. at SSRL[20] and, more recently, by Briand et al. at LURE.[21] Recent work by our group resulted in the observation of the radiationless analog of this process, i.e., the Auger resonant Raman effect (Fig. 3).[22] Threshold excitation of x-ray spectra has been used by Deslattes et al. to identify satellites resulting from multiple excitation.[23] Experiments of this nature strain the limits of resolution and stability at currently operating facilities. An *ab initio* designed beam line for atomic physics at NSLS is likely to incorporate improvements that will open this important field to extensive experimentation.

3. Some Desirable Beam-Line Features for High-Energy Atomic Physics Research

A few features that would clearly be of value for work with hard synchrotron radiation are listed here.

i) High resolution:

Small beam diameter to reduce source size.

Beam-steering by x rays (not UV) to hold source position.

Interchangeable Bragg crystals and planes, to allow work near $\theta \approx \pi/2$ (because $\Delta E/E = \mathrm{ctn}\theta\Delta\theta$).

Availability of tables showing fluxes and $\Delta E/E$.

Ability to monitor Bragg-crystal temperatures.

ii) Facilities to readily monitor flux and polarization.

iii) Good, elaborate software, including temperature input.

iv) Fast time pickoff to gate.

v) Ample space around stations.

*Work supported in part by the U. S. Air Force Office of Scientific Research (Grant No. 79-0026).

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[6] Physics Today, July 1980, p. 19.

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[16]M. Breinig, M. H. Chen, G. E. Ice, F. Parente, B. Crasemann, and G. S. Brown, Phys. Rev. A 22, 520 (1980).

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[20]P. Eisenberger, P. M. Platzman, and H. Winick, Phys. Rev. Lett. 36, 623 (1976).

[21]J. P. Briand, D. Girard, V. Kostroun, P. Chevallier, and K. Wohrer, in Proceedings of the International Conference on X-Ray Processes and Inner-Shell Ionization (Plenum, New York, in press).

[22]G. S. Brown, M. H. Chen, B. Crasemann, and G. E. Ice, to be published.

[23]R. D. Deslattes, R. E. LaVilla, P. L. Cowan, and A. Henins, in Proceedings of the International Conference on X-Ray Processes and Inner-Shell Ionization (Plenum, New York, in press).

Figure Captions

FIG. 1. Experimental total photon-scattering cross sections of H_2 molecules, compared with independent-particle and correlated theoretical predictions. From Ref. 11.

FIG. 2. Measured Kr absorption spectrum near the K edge and theoretical decomposition. From Ref. 16.

FIG. 3. (a) Measured Xe L_3 absorption edge, decomposed according to Ref. 16. (b) Energies of the L_3-$M_4M_5(^1G_4)$ Auger line and its satellites. Near threshold, the ^1G diagram line is shifted by post-collision interaction (PCI). The satellites are shifted due to screening by 5d and 6d spectator electrons, respectively; their energies exhibit linear (Raman) dispersion. (c) Width of the measured ^1G diagram-line spectrum, as a function of excitation energy. From Ref. 22.

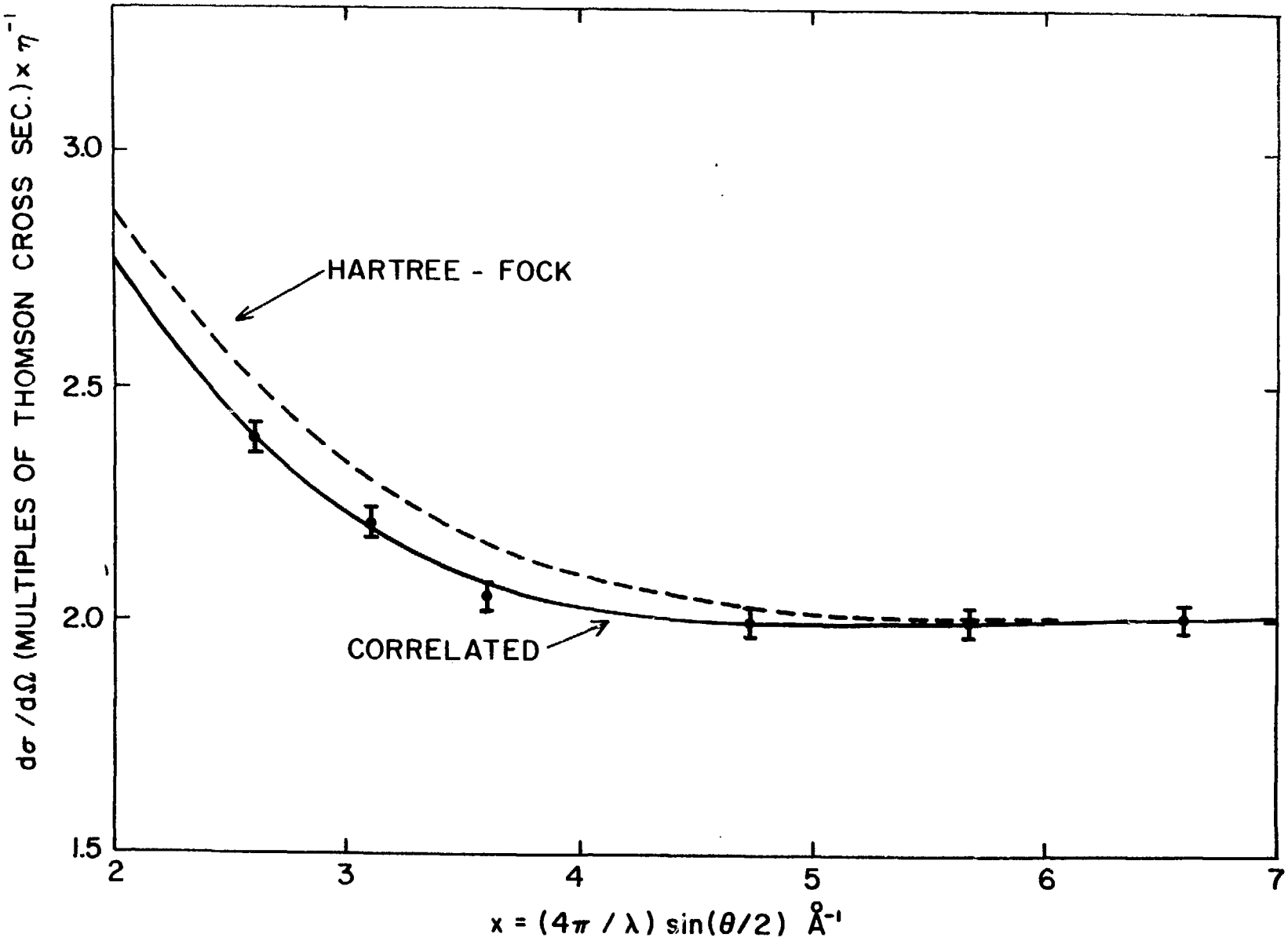
dσ /dΩ (MULTIPLES OF THOMSON CROSS SEC.) × η⁻¹
3.0
2.5
2.0
1.5
HARTREE - FOCK
CORRELATED
2
3
4
5
6
7
x = (4π / λ) sin(θ/2) Å⁻¹

Fig. 1

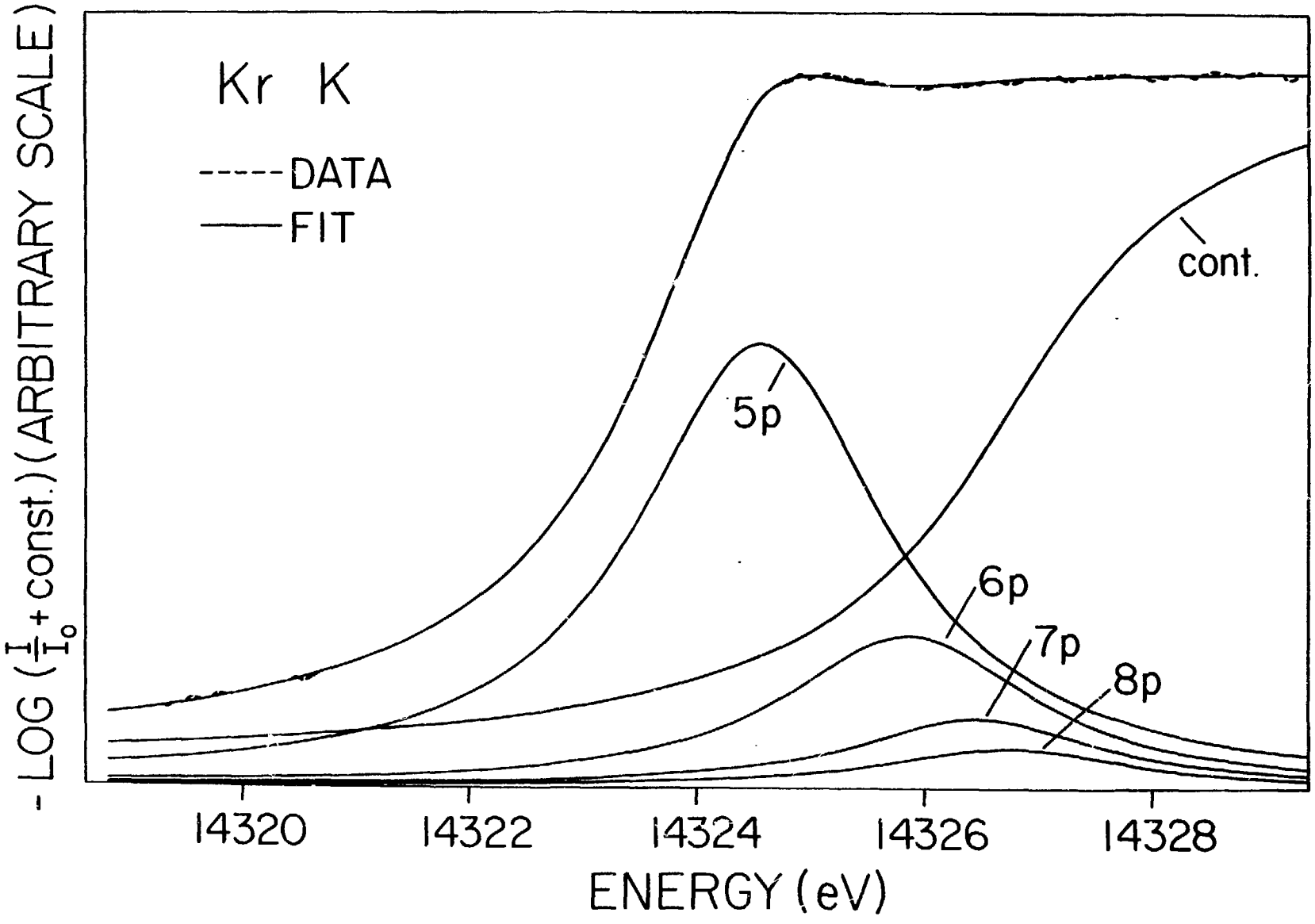
Kr K
-----DATA
——FIT
cont.
5p
6p
7p
8p
- LOG ($\frac{I}{I_o}$ + const.) (ARBITRARY SCALE)
14320
14322
14324
14326
14328
ENERGY (eV)

Fig. 2

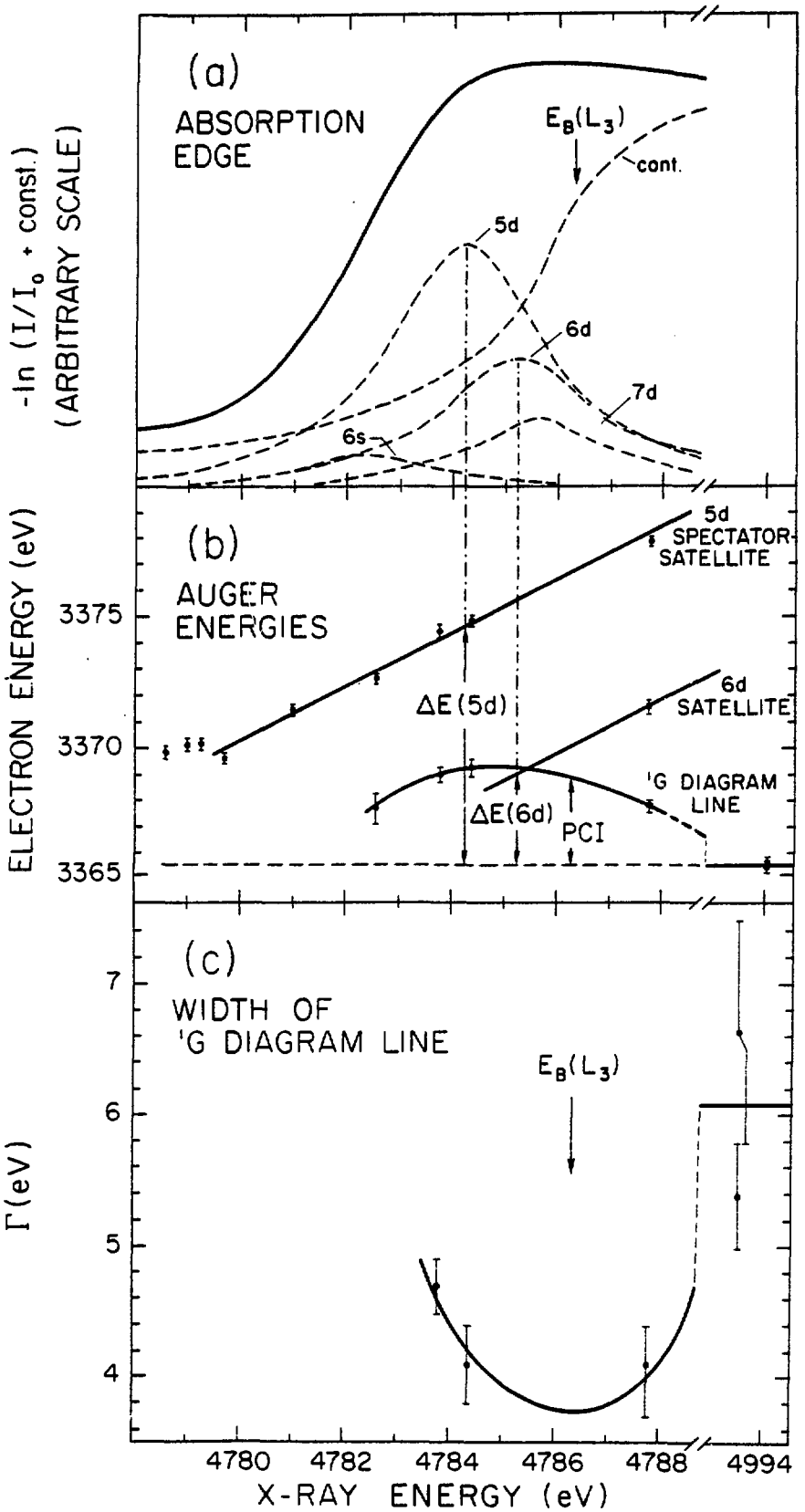
(a)
ABSORPTION EDGE
$E_B(L_3)$
cont.
5d
6d
7d
6s
-ln (I/I$_o$ + const.)
(ARBITRARY SCALE)
(b)
AUGER ENERGIES
5d SPECTATOR-SATELLITE
6d SATELLITE
ΔE(5d)
ΔE(6d)
PCI
'G DIAGRAM LINE
ELECTRON ENERGY (eV)
3375
3370
3365
(c)
WIDTH OF 'G DIAGRAM LINE
$E_B(L_3)$
Γ(eV)
7
6
5
4
4780
4782
4784
4786
4788
4994
X-RAY ENERGY (eV)

Fig. 3

PHOTOIONIZATION OF EXCITED STATES, IONS AND OPEN-SHELL ATOMS: INNOVATIVE SYNCHROTRON EXPERIMENTS*

Steven T. Manson

Department of Physics and Astronomy
Georgia State University
Atlanta, Georgia 30303

The development of synchrotron light sources with increased photon flux in the region 10 eV $\leq h\nu \leq$ 1000 eV opens the door to many atomic physics investigations which have not been possible up to now. In this paper, three general types of experiments will be discussed, each of which offers attractive possibilities for significant advances in our understanding.

Photoionization of Excited States

The study of photoionization of excited states of atoms is virtually virgin territory; only a handful of experimental and theoretical papers on the subject are extant. For photoionization of ground state atoms, whose radii are $\sim a_0$, the Bohr radius, we can learn about the continuum wave function only this region. For excited states, on the other hand, we can get information about the continuum wave function over a much larger region than is accessible from a ground state owing to the much larger physical size of an excited state. In addition, owing to its size, the phenomenology of the photoionization cross sections and photoelectron angular distributions turn out to be rather different than ground states. For example, it is fairly well established that Cooper minima,[1] zeroes in the dipole matrix element, occur for ground states only for outer subshells whose wave functions have nodes and $\ell \rightarrow \ell + 1$ channel and then

never more than one for a given case. For excited states, theory predicts[2] that for the excited 5d state of Cs, for example, there are two minima in the $d \rightarrow f$ channel and one in the $d \rightarrow p$. Now this is not an isolated case and there are many predictions of such phenomena for excited states of atoms[3] but, to date, there is no experiment either confirming or denying these predictions.

An experimental test could be envisioned with a beam of Cs atoms being crossed by a laser to excite some of them to a particular state, then being ionized by the synchrotron light. The use of synchrotron light, rather than a line source, is crucial since the cross sections need investigation over a broad photon energy range. Such an experiment would require photoelectron detection to separate out ground and excited state ionization, and angular distribution work would also be possible (and valuable).

Photoionization of Atomic Ions

The photoionization of atomic ions has received a significant amount of theoretical attention[4,5] owing to the fact that there is almost no experimental work[6,7] and due to its importance in various areas, e.g., astrophysics. Theory predicts, among other things, that inner shell cross sections for ions are unaffected by outer electron removal.[4,5,8] This prediction, along with the general degree of accuracy of these calculations certainly need to be tested over a broad range of photon energy for at least several cases.

Such an experiment would probably involve a beam of ions, perhaps with a mass spectrometer to remove other charge states. The technique of Lucatorto and McIlrath[6,7] might be used to create the ions in the

first place.

Photoionization of Open-Shell Atoms

Of the over one hundred elements in the periodic table, only a dozen or so are closed-shell atoms; the rest have open shells. Nevertheless, over 95% of the experimental work on atomic photoionization has been carried out on closed-shell atoms, particularly the noble gases. Aside from the fact that the paucity of data for open-shell atoms requires experimental work to benchmark theory, there is a whole extra dimension to open-shell atoms. Namely, the open shell(s) admit of various angular momentum couplings (multiplet structure). Thus photoionization of Cℓ $(3p^5)^2P$, for example, can go to Cℓ$^+$ $(3p^4)$ $^1D, ^1S, ^3P$, three possible states[9]. Experimental studies of the cross sections to each of the final ionic states, as well as their ratios, would greatly advance our understanding of the process. At present, there exist a number of theoretical cross sections[10]; experiment is required to tell which, if any, are correct.

In addition, photoelectrons leaving an open-shell atom do not "see" a central field, as is the case for closed-shell atoms. The non-central, or anisotropic, field can exert a torque, thus allowing for the possibility of angular momentum exchanges between the photoelectron and the ionic core. This, in turn, leads to dramatic effects in the photoelectron angular distributions, particularly for atomic s-electrons. A particularly striking example has been found for Cℓ 3s photoionization[11] where, at certain energies, instead of the expected $\cos^2\theta$ distribution, a $\sin^2\theta$ distribution is predicted.

An experiment would require the synchrotron light to intersect an

atomic Cℓ beam. Electron spectroscopic detection would be required to isolate the particular transition(s) under scrutiny as well as for angular measurements. A tunable light source (a synchrotron) is required since the energy dependence of cross sections, branching ratios, and angular distributions are of the greatest interest.

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ATOMIC STRUCTURE AND ELECTRON CORRELATIONS*

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I. INTRODUCTION

Synchrotron experiments combined with theoretical calculations have already given much information on atomic structure and the effects of electron correlations, and this combination of theory and experiment is expected to yield much new information in coming years. In the calculations of photoabsorption cross sections, it is almost always necessary to include electron correlations in both initial and final states to obtain good agreement with experiment.

The main theoretical approaches which include effects of electron correlations have been R-matrix theory[1], random phase approximation with exchange (RPAE),[2,3] relativistic random phase approximation with exchange,[4] and many-body perturbation theory (MBPT).[5]

Reviews of experimental and theoretical work may be found in the book edited by Wuilleumier[6] and in recent proceedings of the International Conferences on Vacuum Ultraviolet Radiation Physics.[7-9] Excellent review articles on atomic photoionization experiments and theory have been written recently by Samson[10] and Starace.[11]

II. SINGLE PHOTOIONIZATION CROSS SECTIONS

In this section, a very brief discussion is given of single-photoionization cross sections where a photon is absorbed and one electron

is ejected. This is in contrast to the case of photoionization with excitation where one electron is ejected and a second electron is either ejected (double photoionization) or excited to a higher-lying bound orbital.

Most calculations of photoionization cross sections including correlations have been on closed-shell systems including the rare gases. Calculations have also been made on selected open-shell atoms with $Z \leq 17$ as described in the review articles already quoted. Experiments on open-shell atoms have also been limited, although synchrotron measurements of absolute cross sections of metallic vapors by Sonntag and coworkers[12] and relative cross sections of metallic vapors by Connerade and co-workers[13] are of great interest. Important work on open-shell atoms is also being done by the group at the Harvard College Observatory.[14-16]

A number of theoretical calculations were recently completed on the neutral chlorine atom and are compared in Fig. 1. Hartree-Fock calculations are too high in the threshold region and final state correlations involving mixing of the $3p^4$ multiplets are important. For example, mixing such as $3p^4\ {}^3P\ kd\ {}^2D$ with $3p^4\ {}^1D\ k'd\ {}^2D$ is important in the ${}^2D$ channel. Open-shell RPAE calculations are by Starace and Armstrong[17] (not including mixing of different $3p^4$ multiplets) and by Cherepkov and Chernysheva;[18] R-matrix calculations are by Lamoureux and Combet-Farnoux;[19] many-body perturbation calculations are by Brown et al.[20]; and close-coupling (length) calculations are by Conneely.[21] Resonances leading to all edges other than the lowest have also been calculated.[19,20]

Calculation of the 3s cross section for chlorine illustrates a typical correlation effect which occurs when the absorption oscillator

strength to the continuum is small for the subshell being observed but there is a neighboring subshell with strong absorption to the continuum. Figure 2 shows the calculated σ_{3s} for chlorine. The curves labelled HFL and HFV are Hartree-Fock length and velocity curves, respectively. When correlations are included, there is a strong qualitative change in the cross section. The largest effect is due to mixing of $3s^2 3p^4 kd$ and $3s^2 3p^4 ks$ into the $3s3p^5$ kp final state. This effect may also be described by saying that the photon is absorbed first by a 3p electron and then by coulomb correlation the excitation is transferred to a 3s electron, the original 3p electron being deexcited. This process depends both on 3p continuum oscillator strengths and correlations between the 3s and 3p subshells.

A simple system which shows strong correlation effects is the zinc atom $3d^{10}4s^2$. Experimental[22] and theoretical[23] results have been obtained for the photoionization cross section of the $(4s)^2$ subshell and are shown in Fig. 3. The curves labelled HFL and HFV are Hartree-Fock length and velocity curves and are the lowest-order cross sections in a many-body calculation. Near threshold the HFL curve is almost twenty times larger than experiment, indicating very large correlation effects. The curves labelled NRL and NRV are length and velocity curves which include effects of correlations except for those leading to the $3p \rightarrow np$ resonances. These are admixtures of $4s^2 3d^9 np\,^1P$ configurations into the $3d^{10}4skp\,^1P$ final states. When these effects are included, the final curve VCF is obtained which is the velocity-correlated-frozen core curve. The frozen core designation indicates that excited kp orbitals were calculated in the fields of $3d^9 4s$ where the 3d and 4s are Hartree-Fock

orbitals for the neutral atom. The curve VCI was obtained using kp orbitals calculated in the relaxed field of the zinc ion. In both case the length curves are very close to the velocity results but are not shown. Figure 4 shows the cross section in the region of the 3d → 4p resonance. Spin orbit effects cannot be neglected and there are three interacting resonance states $3d^9 4s^2 4p\,^1P_1$, $^3P_1$, and $^3D_1$. The absorption window between the two large resonances is obtained in calculations only when interactions between resonances are included.

Other resonance structure in atoms which is of considerable interest involves inner shell excitation to partially filled shells. Interesting examples of this occur in transition metal elements scandium to nickel where there is interesting resonance structure[12,24,25] in the 3d and 4s partial cross sections due to 3p → 3d resonance transitions. It would be interesting to measure this type of structure in other atoms. References for other atoms with, for example, partially filled 4f shells may be found in the review by Samson.[10] It would be particularly helpful to have measurements of partial cross sections to gain a complete understanding of these phenomena. For example, the 3p partial cross sections for transition metal elements would be of interest.

III. PHOTOIONIZATION WITH MULTIPLE EXCITATION

Because of the many-electron character of atomic states, it is possible for a photon to be absorbed and have one or more electrons ejected and others excited. There has been very little work so far on these processes, particularly in measuring cross sections as a continuous function of photon energy. These cross sections can be surprisingly large, approaching 50% of the total cross section (e.g. for Xenon) in certain energy ranges for double photoionization cross sections[10]

in which two electrons are ejected. This process has been studied recently for the rare gases in regions where the photon energy was too low to eject an inner electron which could result in double ionization via the Auger process.

Existing work on double photoionization has been reviewed by Samson[10] and by Starace.[11] Most of the work has been on the rare gases, both experimental[26-31] and theoretical.[32-33] Chang and Poe[32] calculated the double photoionization cross section for Ne and Carter and Kelly[33] calculated both Ne and Ar. Although both calculations used many-body perturbation theory and agree fairly well with experiment, there is noticeable disagreement between the two calculations on Ne. The many-body diagrams contributing to photoionization with excitation are shown in Fig. 5 for a pair of bound electrons in single particle states p and q being excited to states k, k'. Diagrams should be read from bottom to top. Diagrams (a) - (d) are the lowest-order diagrams contributing to this process and diagrams (e) - (g) represent selected higher-order diagrams which were included in the calculations of reference 33 and had the effect of bringing length and velocity results into slightly better agreement. The heavy dot represents the dipole interaction. Diagrams (a) and (b) represent correlation in the initial state and diagrams (c) and (d) represent correlation in the final state. Comparison of the calculations for Argon with experiment is shown in Fig. 6. The calculations only included correlations among $3s^2 3p^6$. Agreement with experiment is surprisingly good for a low-order calculation. The data of Holland et. al. are particularly interesting as the 2p edge is approached. Since the calculations omitted 2p effects, it is not surprising that they do not show this rise in the region of 240 eV.

If the 2p contributions are included, the major effect is expected from diagram (d) of Fig. 5 with r = 2p and p, q = $(3p)^2$. The 2p electron is ejected virtually, followed by an Auger decay which conserves energy. The diagram of course, becomes resonant when the photon energy reaches the 2p ionization energy. However, the 2p cross section already contributes to the total absorption before the ionization edge due to this Raman-like process. This appears to be analogous to the x-ray Raman scattering observed recently.[34,35] An interesting feature in the double photoionization is the fact that an infinite number of partial waves may contribute. In the argon calculations of reference 33, partial waves kpkd, kskp, kdkf, and kskf were included, with the kpkd contribution being largest. In addition, large contribution to the double cross section came from ejection of 3s3p pairs even though the 3s single cross section alone is small.

It would be very interesting to have many more experiments on double photoionization. Problems which should be studied include contributions of different pairs; studies of cross sections near inner ionization edges and interference with the Auger process; studies of the energy distribution of emitted electrons which should help to identify the Auger contribution; angular distributions of electrons emitted in double photoionization. It would also be interesting to measure x-ray Raman cross sections as functions of hν.

IV. PHOTOIONIZATION WITH BOUND EXCITATION

Very little has been done so far in measuring cross sections in which one electron is ejected and one excited to a bound level. From a theoretical point of view, a very simple approximation to this process

is the Shake theory which has been reviewed by Åberg.[36] However, this approximation is generally inadequate and does not allow for excitations with $\Delta\ell \neq 0$. Recently there has been renewed interest in photoionization of $He(1s)^2 \rightarrow He^+$ (n = 2). Measurements of this cross section have been made recently by Wuilleumier[37] and by Woodruff and Samson.[38] The data of Woodruff and Samson show interesting resonance structure converging on He^+ (n = 3). Experiments so far do not separate out the 2s and 2p contributions which are in very different ratios according to the close-coupling calculation by Jacobs and Burke[39] and a recent many-body calculation by Chang.[40] The calculation by Chang is in good agreement with experiment over a wide range of frequencies but does not show any of the resonance structure.

A very interesting process has been observed recently by Iwan et al. in Cu^+. They find $3p^6 3d^{10} + h\nu \rightarrow 3p^5 3d^{10} 4s \rightarrow 3p^6 (3d^8 4s) + e^-$. This is then a strong resonance in the 3d photoionization with excitation (3d → 4s) cross section. It would be interesting to measure this cross section over a wide range of photon energies including this resonance. There is clearly much work to be done in measuring and calculating many different sections of photoionization with excitation and their angular distributions.

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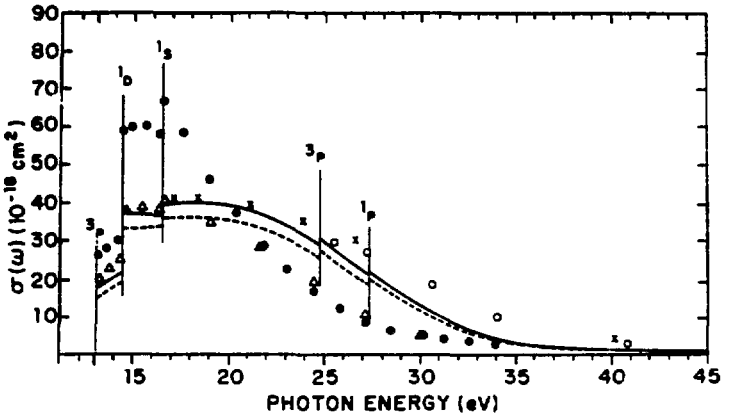

Fig. 1. Calculated photoionization cross sections for neutral chlorine. Solid (dashed) curve represents MBPT dipole length (velocity), Ref. 20. •; RPAE calculation by Starace and Armstrong, Ref. 17. Δ, RPAE calculation by Cherepkov and Chernysheva, Ref. 18. o, R-matrix calculation by Lanoureux and Combet-Farnoux, Ref. 19. x, length close-coupling calculation by Conneely, Ref. 21.

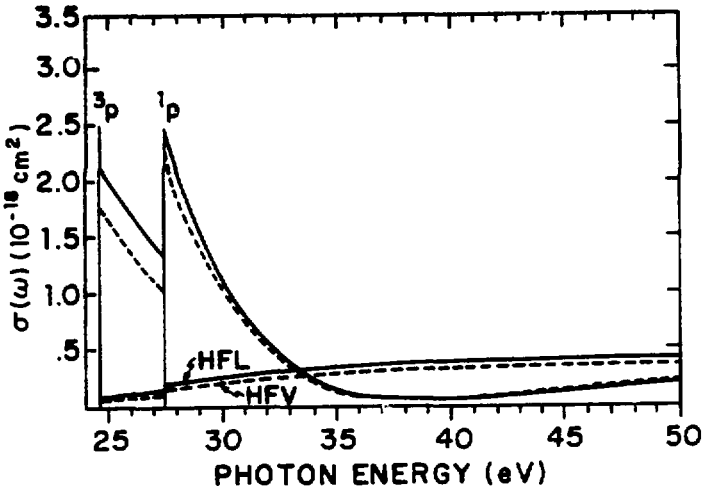

Fig. 2. Total 3s subshell cross-section for neutral chlorine calculated by Brown et al, Ref. 20. Upper curves are length (solid) and velocity (dashed) including correlations. Lower curves are Hartree-Fock length (HFL) and velocity (HFV).

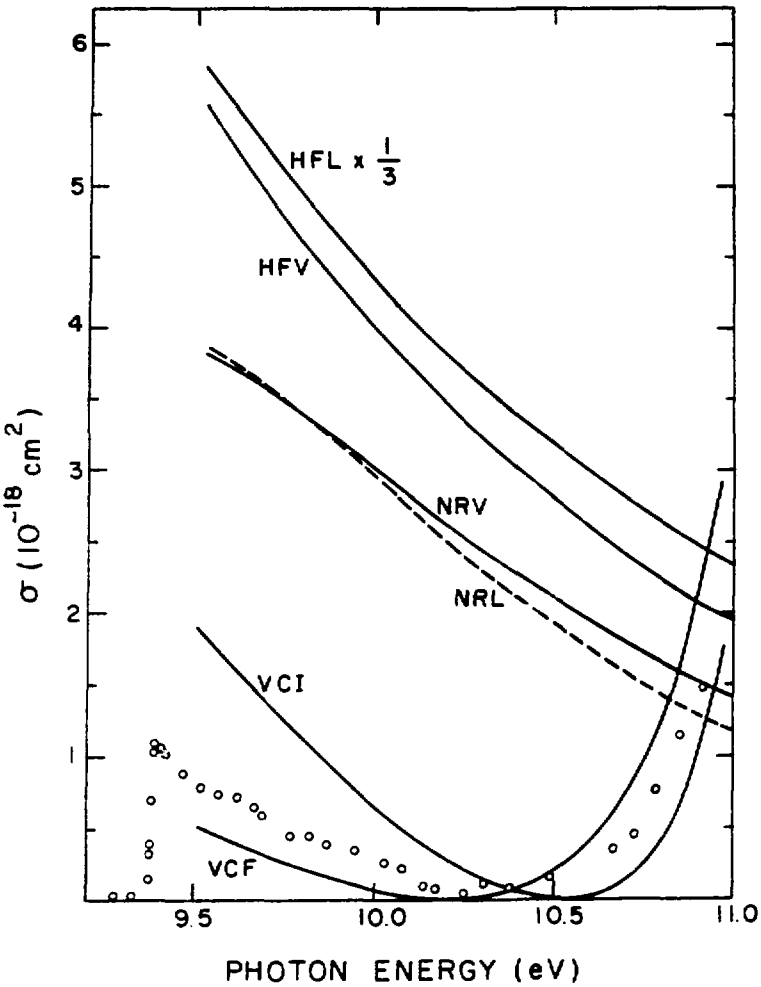

Fig. 3. Cross sections for photoionization of the 4s subshell of neutral zinc calculated in Ref. 23. Curves HFL and HFV represent Hartree-Fock length and velocity cross sections using frozen-core (FC) orbitals. Curves NRL and NRV are correlated length and velocity curves omitting resonance diagrams. Curves VCF and VCI are correlated velocity cross sections with frozen core (1s) and ionic core (I) orbitals respectively. Circles are experimental points by Marr and Austin, Ref. 22.

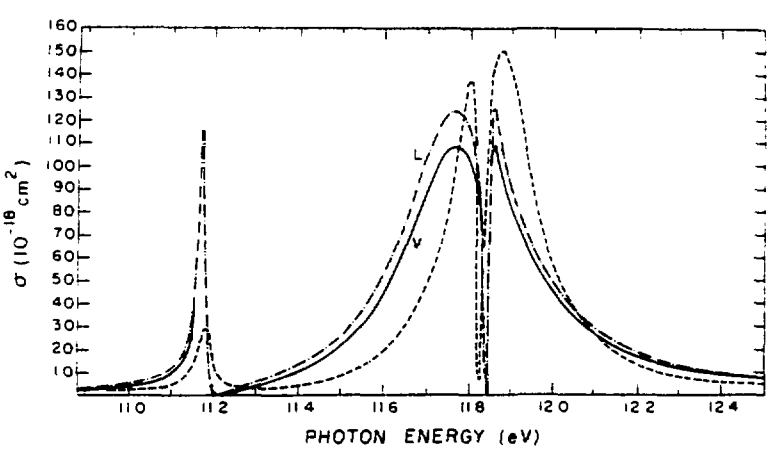

Fig. 4. Photoionization cross section of zinc 4s subshell in the $3d^94s^24p$ resonance region. Solid line (dash-dot line) correlated velocity (length) cross section from Ref. 23. Dashed line, experimental points from Marr and Austin, Ref. 22.

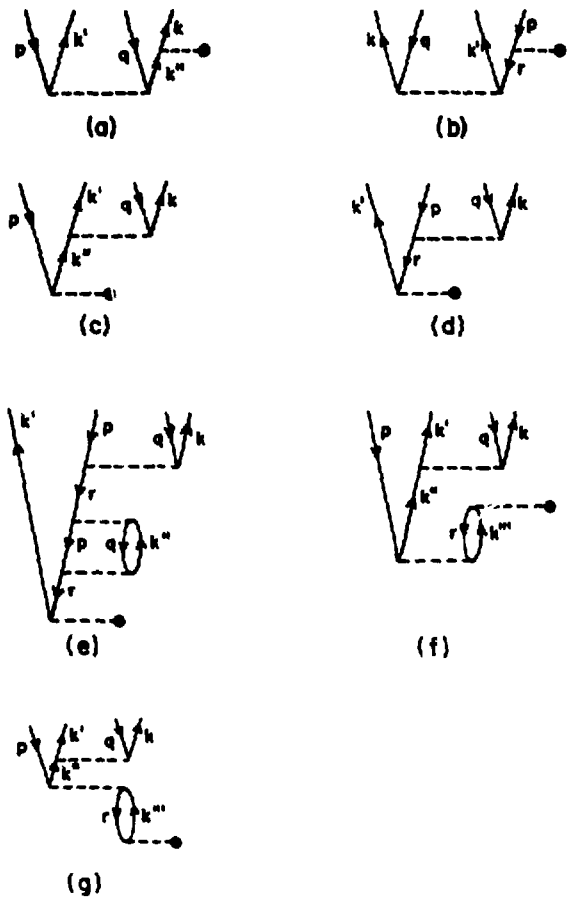

Fig. 5. Diagrams contributing to the double photoionization process. Full circles represent matrix elements of z. Broken lines represent Coulomb interactions.

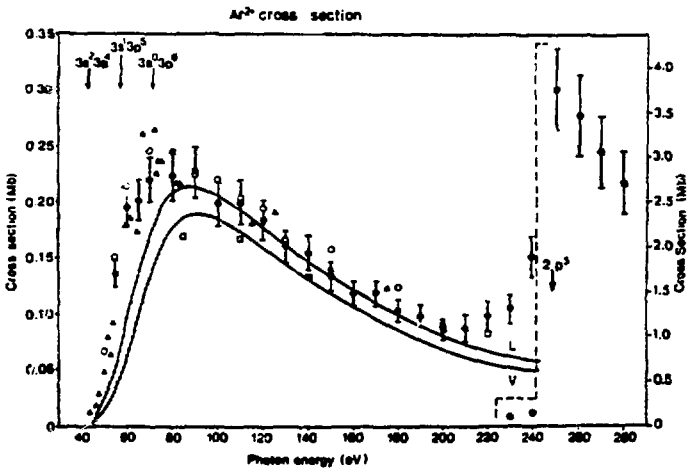

Fig. 6. Double photoionization cross section for neutral argon. Solid curves are dipole length (L) and velocity (V), Ref. 33. Experimental points: ● - Holland et al, Ref. 31.
Δ - Schmidt et al, Ref. 26.
□ - Carlson, Ref. 30.
■ - Lightner et al, Ref. 29.
▲ - Samson and Haddad, Ref. 28.
o - Wight and Van der Wiel, Ref. 27.

Dup

TRANSITION PROBABILITIES FOR ATOMS*

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Current status of advanced theoretical methods for transition probabilities for atoms and ions is discussed. An experiment on the f values of the resonance transitions of the Kr and Xe ieoelectronic sequences is suggested as a test for the theoretical methods.

Accurate transition probabilities for allowed and forbidden transitions of neutral atoms and ions are needed in a wide range of problems in atomic physics, astrophysics, and recently in the diagnostics of high temperature plasmas for magnetic fusion.

Theoretically, the interaction of a photon with an atom or ion is easier to describe than that of charged particles such as electrons and ions. Basically it reduces to calculating a transition matrix element of the form

$$M_{AB} = \langle A | Op | B \rangle \quad ,$$

where A and B are the levels involved in the transition, and Op is an operator representing the multipole transition of interest. The actual form of the operator depends on the degree of sophistication (e.g., relativistic formulation, frequency dependence, etc.); nevertheless it is well defined.[1] The traditional approach is to calculate wave functions for levels A and B separately, and then to evaluate M_{AB} from the wave functions. An alternative approach is to compute M_{AB} directly without producing the wave functions, as is done in the random phase approximation (RPA) and the many-body perturbation theory (MBPT).

In both approaches, the accuracy depends strongly how well the relativistic and electron correlation effects are accounted for. The relativistic effects are important only for medium to heavy atoms, mainly in transitions involving inner-shell electrons, although there are examples of the relativistic effects in the outer shells of heavy atoms.[2,3] In the case of forbidden transi-

tions, relativity can be important even for low Z atoms as in the case of the M1 transitions $1s2s\,2\,^3S_1 \rightarrow 1s^2\,1\,^1S_0$ near the neutral end of the He sequence.[4-7] For the outer shells of neutral atoms and ions of low ionicity, the correlation effects are dominant. Thus, studies of transition probabilities along isoelectronic sequences provide fertile ground for testing various theories of the relativistic and correlation effects.[8,9] Also, such a study readily identifies shifts in coupling schemes that often manifest themselves as level crossings and configuration mixing. Many articles have been published on the behavior of transition probabilities along isoelectronic sequences,[10-14] but I shall focus on the resonance transitions of the Be I sequence to illustrate the relativistic and correlation effects.

In Figure 1, electric dipole oscillator strengths, f, for the $2s^2\,^1S_0 \rightarrow 2s2p\,^{3,1}P^o_1$ transitions of the Be-like ions are presented. The difference between the dotted curve and the lower solid curve as nuclear charge Z increases is due to the relativistic effects such as change in transition energies and contraction of wave functions. Shift from the LS to the jj coupling for high values of Z is responsible for the rise of the f values for the "forbidden" $^3P^o_1$ transitions. Disagreement at Z = 4 among various theoretical values of the oscillator strength results from different degrees of correlation effects accounted for in the theories cited.

For instance, the relativistic RPA results[15] for the $^1P^o_1$ transitions are superior to those from the relativistic multiconfiguration Hartree-Fock (MCHF) method,[10] particularly near the neutral end of the sequence. However, the

two methods produce practically identical results for higher Z values. The results for the singlet transitions from the Bethe-Goldstone method,[16] though not shown in Figure 1, agree closely with the relativistic RPA results. On the other hand, for the triplet transitions, the RPA and the MCHF methods give different values for high Z ions such as Mo^{38+}. With the RPA method, the results for forbidden transitions are less reliable than those for allowed transitions.

The standard RPA method uses a single-determinant HF wave function as a starting point. As a result, the transition energies (or ionization potentials for photoionization) are not as reliable as the transition probabilities. The relativistic MCHF method can give better transition energies but it is less reliable than the RPA method in transition probabilities. Development of an RPA method that starts with MCHF wave functions will eventually eliminate most of the problems mentioned above. Current status of the relativistic MCHF, relativistic RPA, and MBPT methods are compared in Table I. At present, the MCHF method has less restrictions and is easier to use, but the results are less accurate than those obtained from the other methods.

Finally, I would like to mention an experiment that can be done with a synchrotron light source. In neutral Kr and Xe, the $np^6\ {}^1S_0 \rightarrow np^5(n+1)s\ {}^3P^o_1$ transitions are no more "forbidden" than the "allowed" ${}^1P^o_1$ transitions, as can be seen from Table II. The f values for the transitions are affected by the correlation effects both in the valence (5p) and inner (e.g., 4d) shells, and also by relativistic effects such as the spin-orbit interaction. The absolute f

values are not known accurately, experimentally or theoretically. The lifetimes of the P levels are of the order of nanoseconds. Reliable experimental data on the f values or lifetimes for the resonance lines of Kr I and Xe I sequence—particularly near the neutral end—will help to test existing and new theories.

The author wishes to thank Professor W. R. Johnson and Dr. K. T. Cheng for valuable discussions.

Table I. Current Status of Advanced Theories for Transition Probabilities

	MCHF	RPA	MBPT
Open shell	yes	not yet	yes, in principle
Relativity	yes	yes	not yet
Continuum correlation	indirect, difficult	direct, RPA equation	direct, brute force
Gauge invariance	no	yes	depends
Accuracy	good	better	best, in principle
Isoelectronic sequences	yes	yes, but limited	not yet

Table II. Dipole Oscillator Strengths for the $np^6\ {}^1S_0 \rightarrow np^5(n+1)s\ {}^{3,1}P_1^o$ Transitions of Kr and Xe.

	Kr		Xe	
Level	$^3P_1^o$	$^1P_1^o$	$^3P_1^o$	$^1P_1^o$
Excitation energy, eV	10.03	10.64	8.44	9.57
f values				
Theory				
Relativistic Hartree-Fock[17]	0.222	0.175	0.312	0.168
Effective operators[18]	0.176	0.177	0.246	0.268
Experiments				
Lewis[19]	0.204	0.184		
Wilkinson[20]	0.159	0.135	0.260	0.270
Chashchina and Schreider[21]	0.21	0.21	0.28	0.23
Wieme and Mortier[22]			0.214	0.180
Electron impact[23]	0.173	0.173	0.26	0.19
Electron impact[24]			0.183	0.169

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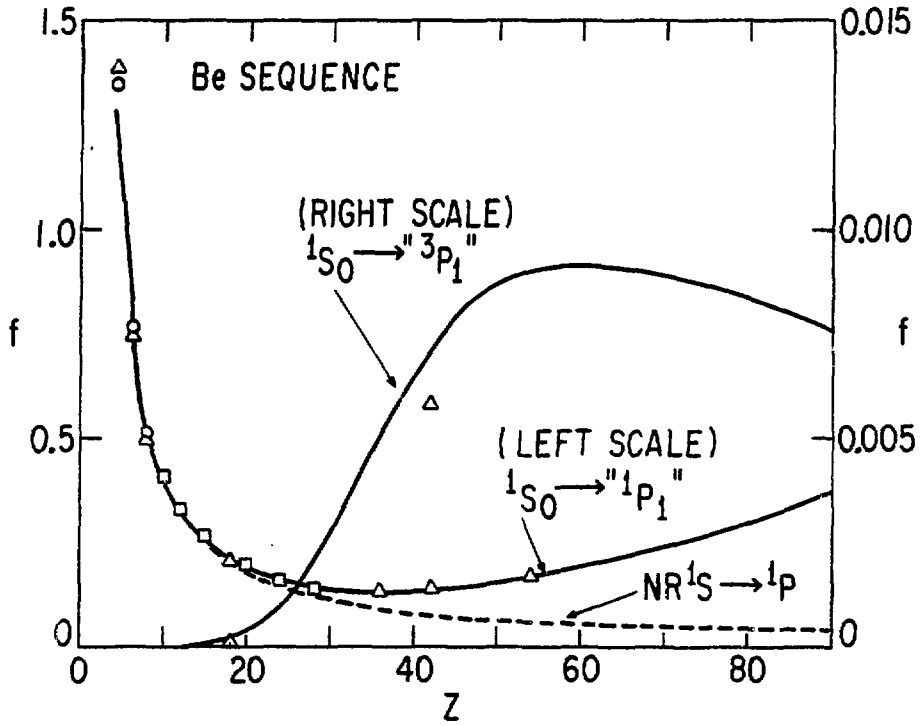

FIG. 1.--Dipole oscillator strengths for the $np^6\ {}^1S_0 \rightarrow np^5(n+1)s\ {}^{3,1}P_1^o$ transitions of the Be sequence. The solid curves are the relativistic MCHF results (Ref. 10), the dotted curve is the non-relativistic MCHF results (Ref. 10), the triangles are the relativistic RPA values (Ref. 15), the circles are those from non-relativistic configurationa-mixing calculations by Sims and Whitten (Ref. 25), and the squares are the values recommended by Smith and Wiese (Ref. 26). Note the different scales for the triplet and singlet transitions.

PHOTOELECTRON SPECTROSCOPY AND PHOTOIONIZATION EXPERIMENTS ON ATOMS AND FREE MOLECULES*

Thomas A. Carlson

The purpose of this exposition is to present a bird's eye view of the value of using synchrotron radiation in the fields of photoelectron and ion spectroscopy of gases. To accomplish this task in the shortest space possible, I have resorted to an outline and tabular form, accompanied by brief commentary.

Nature of Photoelectron Spectroscopy

The power of photoelectron spectroscopy is that it separates out the various transitions between a neutral and single ionized species according to energy. The observed photoelectron peaks can be characterized as due to the ionization of the various atomic and molecular orbitals or due to the various final state effects such as electron shake up and excited vibrational states. In the past, photoelectron spectroscopy has used energy analysis to create one of the most important experimental foundations for the study of the electronic structure of atoms and molecules. But photoelectron spectra also contains information besides energies, namely intensities which are related to photoelectric cross sections. These cross sections, being a function of photon energy, require the intense continuous, polarized source that synchrotron radiation provides.

In atoms the interest in photoelectric cross sections revolves mainly about the many body problem, both in the description of electron correlation in the

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bound state atoms and ions and in the dynamics of the photoionization process. In molecules great interest lies in characterizing molecular orbitals, which unlike atomic orbitals, are in many cases still described in terms that fall far short of even a Hartree Fock solution. In addition photoionization offers the first fundamental step towards understanding chemical reactivity.

Fields Other Than Photoelectron Spectroscopy to be Covered

A. Auger Electron Spectroscopy

B. Ion Spectroscopy

Auger electrons are measured in the same spectrometer as photoelectrons and obviously deserve consideration. Ions produced in the photoionization process can also provide valuable information. In this report we shall concentrate attention on the effects of core shell ionization.

Energy Ranges

A. Valence Shell (10-100 eV)

B. Penultimate Core Levels (100-1000 eV)

C. Deeper Core Levels (1-30 KeV)

D. Modification of Energy Range

1. Wigglers (low energy source $\longrightarrow$ high energy source)

2. Undulators (high energy source $\longrightarrow$ very intense low energy source)

The matching of the research needs to the appropriate range of photon energies is one of the essential concerns of this group. I personally feel that at least 90% of the most important experiments to be done with photoelectron spectroscopy will require photon energies in the range from 10-1000 eV.

Specific Research Areas and Related Problems

A. Photoelectron Spectroscopy

Atoms

1. Cross Sections
   a. total
   b. partial
   c. differential (β parameter)
   d. spin polarized
2. Type of Atom
   a. closed shells
      i. rare gases
      ii. alkaline earths
   b. open shells
      i. nobel metals
      ii. transition metals
      iii. rare earths
3. Final State Effects
   a. autoionization
   b. electron shakeup
4. Core Shell Threshold Effects
5. Shape Resonance
6. Level Widths (lifetimes)
7. Post Collisional Effects
8. Relativistic Effects
   a. high Z
   b. high energy
9. Breakdown in Dipole Approximation

Molecules

1. Cross Sections
   a. total
   b. partial
   c. differential (β parameter)
   d. relative to orientation of molecular axis
2. Size of Molecule
   a. diatomic
   b. triatomic
   c. polyatomic
   d. clusters
3. Final State Effects
   a. autoionization
   b. electron shakeup
   d. vibrational states
      i. branching ratios
      ii. β values
4. Core Shell Threshold Effects
5. Shape Resonance
6. Rotational States
7. Theoretical Basis for Calculating molecular cross sections
   a. MSX_{α}
   b. other methods

B. Auger Electron Spectroscopy

1. Use in Cross Section Evaluation

2. Electron Shakeoff

3. Changes of Spectrum at Threshold

   a. transition probabilities

   b. angular dependence

4. Coincidence with PES

C. Ion Spectroscopy

1. Charge Spectrum as Function of Photon Energy

   a. vacancy cascade

   b. electron shakeoff

2. Molecular Fragmentation

3. Recoil Energy of Ion

4. Coincidence

   a. with photoelectron

   b. with Auger electron

5. Total Cross Section

6. Collisional Neutralization

D. Preparation of Sample

1. Molecular and Atomic Beams

2. Super Sonic Nozzle

   a. removal of Doppler Effect

   b. production of rotational ground state

3. Laser Excitation

4. Metal Vapor

5. High Boiling Molecules

6. Circularly Polarized Light

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POSSIBLE APPLICATIONS OF SYNCHROTRON RADIATION TO X-RAY ASTROPHYSICS

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As the instrumentation for observations in high energy astrophysics has grown increasingly sophisticated, so too has the need developed for improved calibration techniques and facilities. Contemporary satellite-borne observatories contain high resolution spectrometers, polarimeters and x-ray image-forming optics focussed on position sensitive detectors. The Advanced X-ray Astrophysics Facility, a planned free-flying, shuttle-launched x-ray telescope (1.2 m diameter, 10 m focal length), will provide 0.5 arcsecond imagery over a several arcminute field and spectrometry with $E/\Delta E > 1000$ in the energy range 0.1 - 8 keV.[1] Other telescopes in the planning stage include the possibility of $\sim$0.5 arcminute imagery at energies in excess of 100 keV.

I will list here just a few examples from the long list of calibration needs of individual detectors and subsystems.

There is a continuing need for absolute calibration of x-ray transmission diffraction grating efficiencies in the energy range $\sim$0.1 to 2 keV.[2]

In order to improve the design of x-ray grating spectrometers there is a related need for better determination of the optical constants of Au, Cu, Ni and Pt in this energy range.[3]

Imaging instrumentation is being planned for the study of mass flows from and composition of comet nuclei during rendezvous missions.[4] Calibration of these detector systems will require a tunable source of 0.3 - 5 keV x-rays reflected at differing angles from composite targets which model expected comet surfaces.

For diagnostic reasons, some x-ray detectors must be calibrated in intense beams ($>10^3$ $mm^{-2}s^{-1}$) or in the UV. A calibration facility for Bragg crystal polarimeters is an obvious need. Certainly one of the most important measurements in the immediate future will be the study of scattering properties and efficiencies of grazing incidence mirrors.[1]

The problem of calibrating the larger payloads is severe. The facility at Marshall Space Flight Center has or will have a vacuum chamber commodious enough to contain the entire AXAF.[5] This raises the question of the kind of beams available at MSFC and how they compare with synchrotron light sources. The MSFC facility uses a micro focus x-ray tube at the end of a 300m vacuum line 1 m in diameter. They typically fill the aperture with $\sim$1-200 photons $cm^{-2}s^{-1}$. The angular divergence of the beam is 0.5 arcsecond. Obviously this is quite suitable for calibrating imaging optics (and was so used for the HEAO-B X-ray Observatory[6]) although some detectors might be calibrated pixel by pixel.

However, we must bear in mind that only the discrete energies permitted by choice of target are available at MSFC as contrasted with the continuously variable monochromated beams from synchrotron sources. Other advantages of synchrotron facilities include a wider energy range, polarized beams and high luminosity.

Overall it would seem that synchrotron light sources can provide appropriate beams for the design and calibration of instrumentation for high energy astrophysics.

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NSLS MACHINE PARAMETERS AND HARDWARE

Some time was spent during the Workshop on talks by van Steenbergen, Hastings, Howells, Purser, and Radeka which discussed machine parameters, monochromators, ion beam handling, and position-sensitive detectors. We have not reproduced these talks here since their topics, while necessary for stimulating consideration of possible experiments, really lie outside the subject of this Workshop and are covered in detail in other conferences and symposia.

However, it is useful to have handy some general details of the facility so that we do include a summary paper by van Steenbergen and the NSLS staff on the general features of the machine. We have also included a list of the assignments of beam pipes made thus far on the UV and x-ray rings. For current information on the status of the machine and NSLS project and for information on how to become a certified NSLS user consult:

Dr. Roger Klaffky
National Synchrotron Light Source
Building 725B
Brookhaven National Laboratory
Upton, NY 11973

516-345-4974
FTS 666-4974

A detailed listing of useful NSLS reports can be obtained from:

Carolyn Albert
National Synchrotron Light Source
Building 725B
Brookhaven National Laboratory
Upton, NY 11973

The Editors

Proceedings, National Conference on
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June 4-6, 1979, Gaithersburg, MD
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BNL-26250

The National Synchrotron Light Source

Basic Design and Project Status*

by

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Abstract

A summary description and the basic design parametars of the National Synchrotron Light Source, a facility for the generation of intense synchrotron radiaction in the VUV and X-ray range is presented, the parameters of the sources are given, the presently planned facility beam lines are tabulated and the status of the project is indicated.

*Research supported by the U.S. Department of Energy.

Introduction

Interest in the utilization of synchrotron radiation for research in the domain of the material sciences, atomic and molecular physics, biology and technology has grown dramatically in recent years. At Brookhaven National Laboratory this led to the construction, starting in October of 1977, of two high intensity electron storage rings, one with a maximum energy of 700 MeV, for the production of synchrotron radiation in the VUV range, from about 10 Å to the visible region; and one with a maximum energy of 2.5 GeV for the hard X-ray region down to about 0.5 Å, extendable to 0.1 Å by means of high field orbit wigglers. Electron charging of these two storage rings is done using an injector combination consisting of a 100 MeV Linear Accelerator and a 700 Booster Synchrotron. The combination of injector, two high intensity electron storage rings and a multiplicity of monochromatized photon lines comprises the National Synchrotron Light Source. The present parameters and storage ring/accelerator structures are the result of the design effort by the NSLS staff, starting from the basic designs as proposed earlier by Green and Chasman[1].

Description of the Facility

The overall layout of the facility is given in Fig. 1. Electrons, originating from a hot cathode diode gun are accelerated in an S-band linear accelerator to 100 MeV, injected in a multiturn mode into a booster synchrotron[2] and accelerated to 700 MeV. The basic booster structure and injector parameters are given in Fig. 2. After allowing the beam to "damp" at maximum energy in the booster, the beam is transferred either to the VUV[3] or X-ray[4] storage ring. The primary objective of allowing the beam to damp on a "flat-top" in the booster synchrotron is the use of small (vertical) aperture orbit wigglers in either the VUV storage ring, typically for a 50 period undulator[5] for photon source flux enhancement; or the X-ray storage ring, for a high field wiggler for shifting the critical energy to a value of ≈ 25 keV.

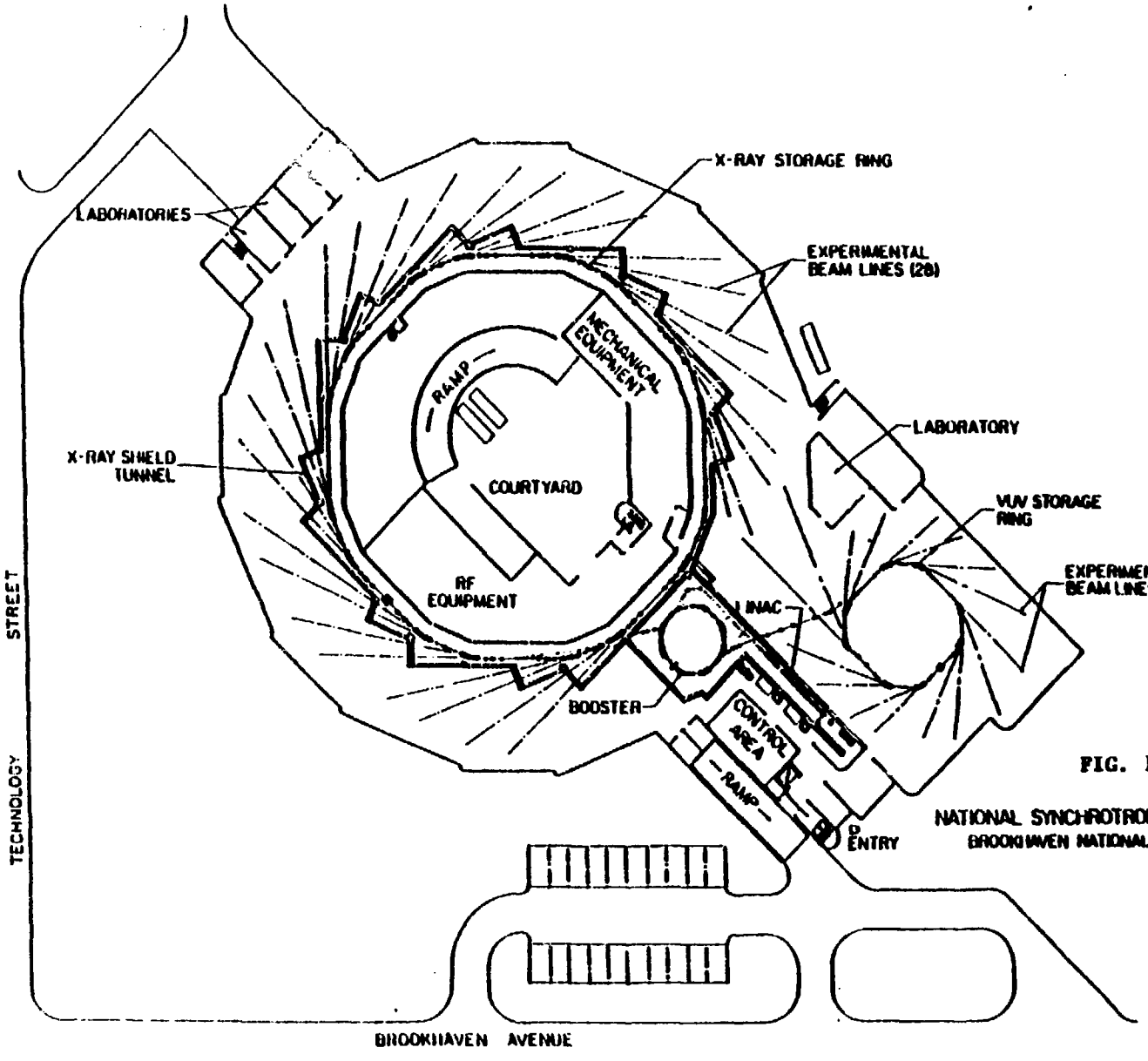


FIG. 1

NATIONAL SYNCHROTRON LIGHT SOURCE
BROOKHAVEN NATIONAL LABORATORY

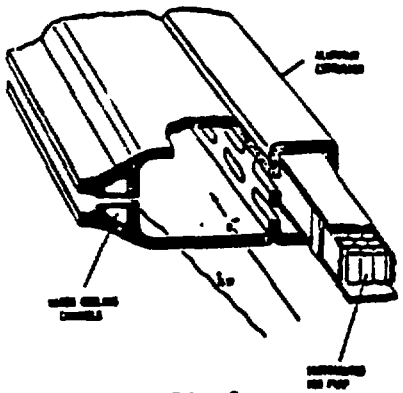
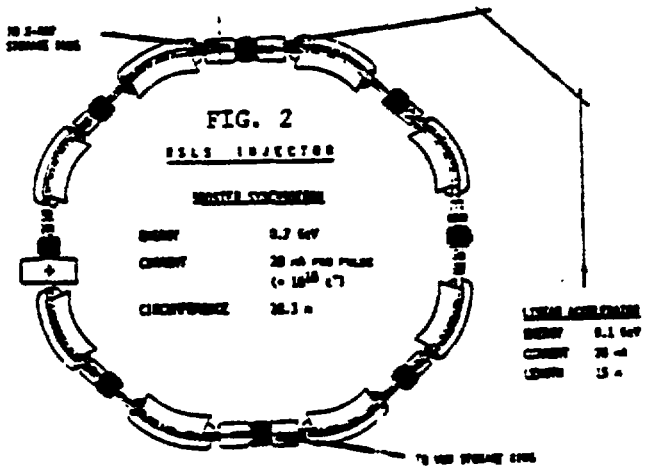


FIG. 3



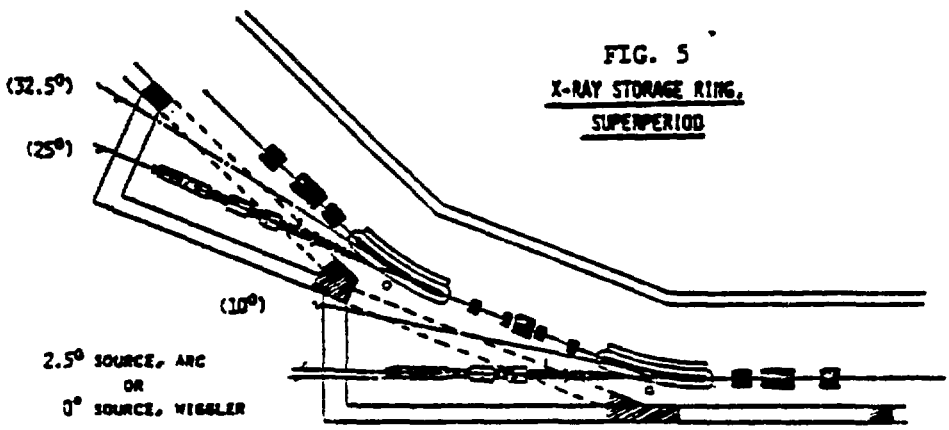


FIG. 5
X-RAY STORAGE RING,
SUPERPERIOD

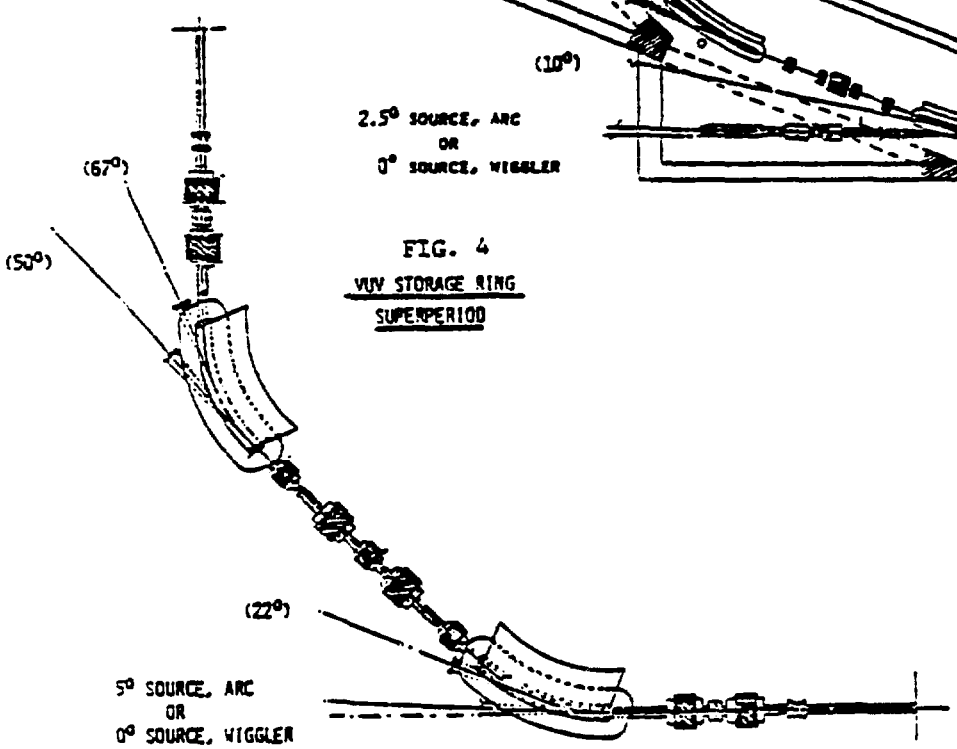


FIG. 4
VUV STORAGE RING
SUPERPERIOD

The charge magnitude in the storage rings is built up by the process of repeated beam transfer from the booster synchrotron, to a value corresponding to 1 Ampere in the VUV ring or 0.5 Ampere in the X-ray ring. In the case of the X-ray ring, the stored charge is increased in energy by acceleration to 2.5 GeV. For the design parameters, the total radiated power in the VUV ring is 11.3 kW and in the X-ray ring = 300 kW, assuming use of 5 high field wigglers in this ring. This demands usage of a vacuum envelope with effective cooling of the area of synchrotron radiation impact. This is achieved by means of an extruded aluminum chamber structure, as shown in Fig. 3. By using two water cooling channels, as shown, greater structural simplicity is obtained in the region of synchrotron radiation ports. This is valid in the VUV ring where a simple slot cut into the vacuum chamber is adequate as a synchrotron radiation port; it is also valid for the X-ray ring where, because of the high caloric density in the radiation exit port crotch, the use of aluminum in this local area must be excluded. Taking advantage of the double cooling channel design a particularly simple copper crotch design has been developed.

Storage Ring Parameters

The VUV and X-ray ring "lattices" are indicated in Fig. 4 and Fig. 5, showing also the locations of the synchrotron radiation ports relative to the ring structures. The basic VUV and X-ray storage ring parameters are given in Table I and Table II. With high beam bunch densities it is anticipated that beam lifetimes (or source brightness lifetimes) will be limited by the Touschek (intrabunch scattering) effect. For the VUV ring, with a stored current of 1 Ampere in 9 bunches and effective bunch length of = 1.1 nsec, the lifetime value is $\gtrsim$ 4 hrs. In the X-ray ring, with a stored current of 0.5 Ampere in 30 bunches and effective bunch length of = 1.6 nsec, the lifetime value at injection is approximately 30 minutes, which is adequate taking into account

TABLE II

X-RAY STORAGE RING PARAMETERS

ENERGY RANGE	2.5 GeV - 0.7 GeV
DESIGN CURRENT	1 A (2 GeV) (3.9 10^{12} e^-)
	0.5 A (2.5 GeV) (1.9 10^{12} e^-)
RADIATED POWER (0.5 A, 2.5 GeV)	252 + $9N_W$ (kW)
λ_c (ϵ_c) AT 1.22 T (B)	2.48 Å (5 keV)
6.0 T (W)	0.5 Å (25.0 keV)
$\tau_{TOUSCHEK}$ (0.7 GeV, 1 A)	$\gtrsim$ 0.6 hrs ($\hat{V}_{RF} \simeq$ 800 kV)
(2.5 GeV, 0.5 A)	$\gtrsim$ 8 hrs (SAME)
$\hat{B}$ (ρ)	1.22 T (6.875 m)
CIRCUMFERENCE	170.08 m
τ_{ORB} (h)	567.7 nsec (30)
DAMPING TIMES (0.7 GeV)	$\tau_x \simeq \tau_y \simeq$ 256 msec; $\tau_\epsilon \simeq$ 129 msec.
(2.5 GeV)	$\tau_x \simeq \tau_y \simeq$ 5.6 msec; $\tau_\epsilon \simeq$ 2.8 msec.
LATTICE STRUCTURE	SEPARATED FUNCTION, TRIPLETS
NUMBER OF SUPERPERIODS	8
LONG STRAIGHTS	4.50 m
MAGNET COMPLEMENT	16 B (2.7 m)
	40 Q (0.45 m)
	16 Q (0.80 m)
	32 S (0.20 m)

TABLE I

VUV STORAGE RING PARAMETERS

ENERGY	0.7 GeV
DESIGN CURRENT	1 A (1.2 10^{12} e^-)
RADIATED POWER (1 A)	11.3 kW
λ_c (ϵ_c)	31.6 Å (390 eV)
$\tau_{TOUSCHEK}$	$\gtrsim$ 4 hrs ($\hat{V}_{RF} \simeq$ 200 kV)
$\hat{B}$ (ρ)	1.2 T (1.91 m)
CIRCUMFERENCE	51.02 m
τ_{ORB} (h)	170.2 nsec (9)
DAMPING TIMES	$\tau_x \simeq \tau_y \simeq$ 21 msec; $\tau_\epsilon \simeq$ 11 msec
LATTICE STRUCTURE	SEPARATED FUNCTIONS, DOUBLETS
NUMBER OF SUPERPERIODS	4
LONG STRAIGHTS	3.26 m
MAGNET COMPLEMENT	8 B (1.5 m)
	24 Q (0.3 m)
	12 S (0.20 m)

TABLE II

X-RAY STORAGE RING PARAMETERS

ENERGY RANGE	2.5 GeV - 0.7 GeV
DESIGN CURRENT	1 A (2 GeV) (3.9 10^{12} e^-)
	0.5 A (2.5 GeV) (1.9 10^{12} e^-)
RADIATED POWER (0.5 A, 2.5 GeV)	252 + $9N_M$ (kW)
λ_c (ϵ_c) AT 1.22 T (B)	2.48 Å (5 keV)
6.0 T (W)	0.5 Å (25.0 keV)
$\tau_{Touschek}$ (0.7 GeV, 1 A)	$\gtrsim$ 0.6 hrs ($\hat{V}_{RF} \simeq$ 800 kV)
(2.5 GeV, 0.5 A)	$\gtrsim$ 8 hrs (same)
$\bar{B}$ (ρ)	1.22 T (6.875 m)
CIRCUMFERENCE	170.08 m
τ_{orb} ($\hbar$)	567.7 nsec (30)
DAMPING TIMES (0.7 GeV)	$\tau_x \simeq \tau_y \simeq$ 256 msec; $\tau_\epsilon \simeq$ 129 msec.
(2.5 GeV)	$\tau_x \simeq \tau_y \simeq$ 5.6 msec; $\tau_\epsilon \simeq$ 2.8 msec.
LATTICE STRUCTURE	SEPARATED FUNCTION, TRIPLETS
NUMBER OF SUPERPERIODS	8
LONG STRAIGHTS	4.50 m
MAGNET COMPLEMENT	16 B (2.7 m)
	40 Q (0.45 m)
	16 Q (0.80 m)
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TABLE I

VUV STORAGE RING PARAMETERS

ENERGY	0.7 GeV
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LATTICE STRUCTURE	SEPARATED FUNCTIONS, DOUBLETS
NUMBER OF SUPERPERIODS	4
LONG STRAIGHTS	3.26 m
MAGNET COMPLEMENT	8 B (1.5 m)
	24 Q (0.3 m)
	12 S (0.20 m)

an acceleration time of 3 minutes; at the operating energy of 2.5 GeV the Touschek lifetime is $\gtrsim$ 8 hrs.

In order to maintain precision control of the synchrotron radiation source locations (and exit angles) an elaborate electron beam closed orbit detection and correction system is incorporated in both storage rings, capable of maintaining source locations to within ± 0.1 mm displacements. It is expected, however, that the short term stability of the beam will be within these limits as a result of incorporation of highly stable power supplies for the storage ring magnet systems and the special design attention paid to the foundation structure of both storage rings.

Source Parameters

The photon flux versus wavelength (or photon energy) spectra for the VUV ring and for the X-ray ring, also with a 6 Tesla orbit wiggler, are given in Fig. 6 and a summary of the experimental parameters are given in Table III. The source arc length indicated here is a nominal value only. Actually, the VUV ring will have eight 75 mrad ports and eight 90 mrad ports. The X-ray ring will make use of 50 mrad ports (2 per magnet) of which each will normally be split in two (or more) branches, subtending typically 10 mrad (or less) per branch. It is planned to have two high field wigglers ready for tests on completion of the NSLS construction project, eventually five high field wigglers will be incorporated in the X-ray storage ring. For a horizontal wiggler, a source extent of 10 mrad is feasible, in case of a vertical wiggler (rotation of the plane of polarization), a source extent of 5 mrad nominal is contemplated. Similarly, for the VUV ring, it is planned to incorporate eventually two coherent wigglers in the structure.

Further detailed parameters of the various arc sources and wiggler sources are given, for the VUV ring, in Table IV; and for the X-ray ring, in Table V,

FIG. 6

SYNCHROTRON RADIATION SPECTRA FOR THE NSLS DESIGN PARAMETERS

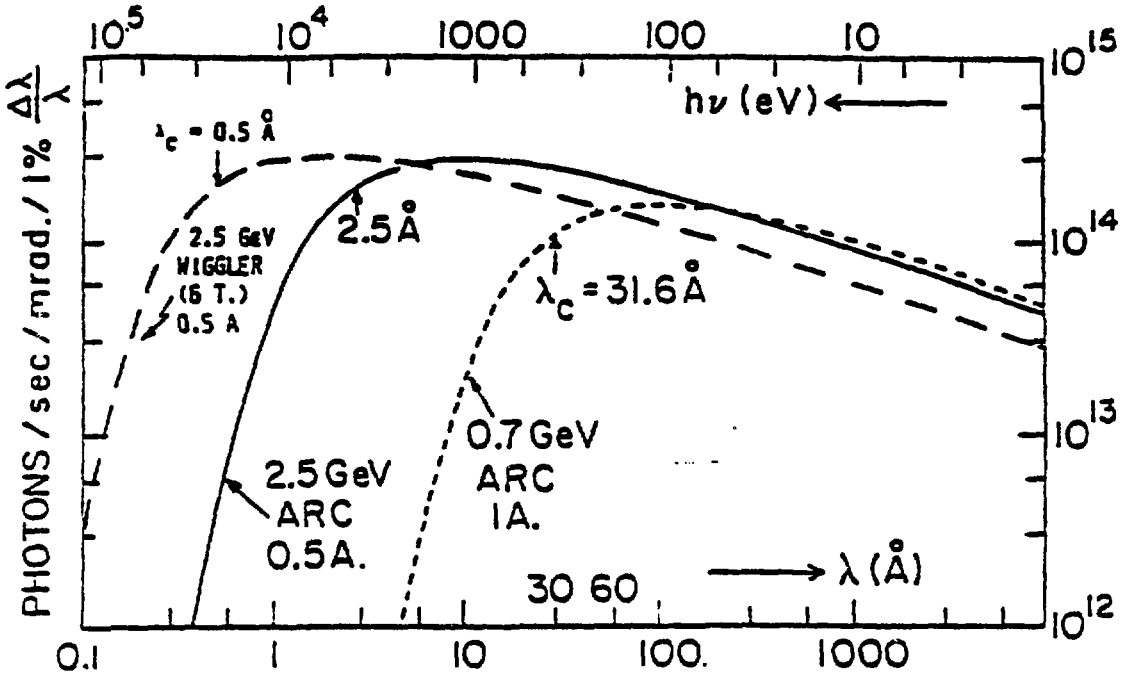

TABLE III

NSLS SUMMARY EXPERIMENTAL PARAMETERS, X-RAY, VUV

	X-RAY (WIGGLER)	X-RAY (ARC)	VUV (ARC)
WAVELENGTH (Å)	1	10	100
[λ_c(Å); ϵ_c(KEV)]	[0.5 ; 25.0]	[2.5 ; 5.0]	[31 ; 0.4]
SOURCE DIMENSIONS			
$2\sigma_Y' \times 2\sigma_{X,T}$ (MM^2)	0.035 x 0.65	0.2 x 0.5	0.2 x 0.55
ARC LENGTH, $\Delta x'$ (MRAD)	5	10	60
VERT. OPENING ANGLE (MRAD) ($2\sigma'$)	0.3	0.4	1.4
FLUX, PER 0.1% $\Delta\lambda/\lambda$ (PH/SEC)	10^{14}	2.5 10^{14}	10^{15}
TIME STRUCTURE			
NUMBER OF BUNCHES	30	30	9
ORBITAL TIME (NSEC)	568	568	170
EFFECTIVE BUNCH LENGTH (NSEC)	1.5	1.7	1.1
BEAM PORTS, MAX.	N($\hat{N}$ = 5)	(28 - N)	16

TABLE V

EXPERIMENTAL PARAMETERS, X-RAY RING

"OPTICS" SOLUTION, E = 2.5 GeV, 10% COUPLING

$\epsilon_x = 8.1\ 10^{-8}$ RAD M; $\epsilon_y = 8.1\ 10^{-10}$ RAD M; $\sigma_\epsilon(\Delta p/p) = 8.2\ 10^{-4}$

SOURCES	$2\sigma_{x,y}$(MM)	$2\sigma_y$(MM)	$N_\gamma(\lambda)$ (PH/S/MRAD/0.5 A/1% $\Delta\lambda/\lambda$)
XW1	0.65	0.035	
WIGGLER SOURCES; $\lambda_c = 0.5$ Å, $\hat{B} = 6$T; $\epsilon_c = 2.5$ keV			$2\ 10^{14}$ AT $\lambda = 1$ Å (12.3 keV) $4\ 10^{13}$ $\lambda = 0.2$ Å (62 keV) $3\ 10^{12}$ $\lambda = 0.1$ Å (123 keV)
B(2.5°)	0.9	0.25	
B(10°), B(32.5°)	0.5	0.2	
B(2.5°)	0.7	0.2	
ARC SOURCES; $\lambda_c = 2.5$ Å, $\hat{B} = 1.2$ T; $\epsilon_c = 5$ keV			$2.5\ 10^{14}$ AT $\lambda = 10$ Å $3.2\ 10^{13}$ $\lambda = 1$ Å $6.0\ 10^{13}$ $\lambda = 4000$ Å

TABLE IV

EXPERIMENTAL PARAMETERS, VUV RING

"OPTICS" SOLUTION, E = 0.7 GeV, 10% COUPLING

$\epsilon_x = 8.7\times10^{-8}$ RAD.M; $\epsilon_y = 8.8\times10^{-10}$ RAD.M; $\sigma_\epsilon(\Delta p/p) = 4.4\times10^{-4}$

SOURCES	$2\sigma_{x,y}$(MM)	$2\sigma_y$(MM)	$N_\gamma(\lambda)$ (PH./S/MRAD/1A/1% $\Delta\lambda/\lambda$)
B (5°)	0.8	0.2	
B(22°), B(67°)	0.65	0.2	
B(50°)	0.55	0.2	
ARC SOURCES; $\lambda_c = 31$ Å, $\hat{B} = 1.2$ T; $\epsilon_c = 0.4$ keV			1.9×10^{13} AT $\lambda = 10$ Å 1.5×10^{14} AT $\lambda = 100$ Å 6.5×10^{13} AT $\lambda = 4000$ Å
UCW	2.0 ($2\sigma_x$=0.15 MM.)	0.15 ($2\sigma_y$=0.025 MM.)	$N_\gamma(\lambda)$(PH./S/1A/1% $\Delta\lambda/\lambda$)
UNDULATORS; $B_0 = 0.4$ T, $\lambda_u = 5$ CM, $N = 50$; $g = 3$ CM, K = 2			k=1; $8\ 10^{16}$ AT $\lambda = 400$ Å k=3; $6\ 10^{16}$ $\lambda = 133$ Å

indicating the very substantial photon flux values (and inherent brightness values) available from these two storage rings ranging from the ≈ 0.1 Å (≈100 keV) value to the visible region.

The basic storage ring lattices have been optimized to achieve optimum source brightness values at the various source locations in the storage ring structures. It should be realized, however, that the source dimensions stated are theoretical values, which do not take into account undetermined, but possible, beam enlargement due to collective effects within the high density electron beams or limited (by feedback systems) beam growth as a result of beam-environment interaction at these high bunch densities. In this respect, it should be stated that various beam optical modes are possible, and have been explored to a certain extent for the storage rings, emphasizing either optimum brightness (at possibly somewhat reduced photon flux) or maximum photon flux from the source (with possibly somewhat reduced brightness).

Experimental Facilities

As part of the NSLS construction phase, four instrumented photon lines will be built for the X-ray storage ring and four lines will be constructed for the VUV ring. These will be optimized for specific research objectives such as small angle scattering studies of biological structures, general X-ray spectroscopy (EXAFS), X-ray diffraction, etc.; and, angle resolved photoelectron spectroscopy of solids, gas phase spectroscopy, fluorescent lifetime studies, etc. The plans for these eight beam lines, as listed in Table VI, are well advanced and descriptions of basic characteristics (wavelength range, resolution, photon flux versus wavelength, area illumination at the "target" station, etc.) are available[6,7]. Detailed designs of specific photon lines are progressing and, typically, a tentative layout of experimental lines around the VUV ring, as shown in Fig. 7, has been arrived at.

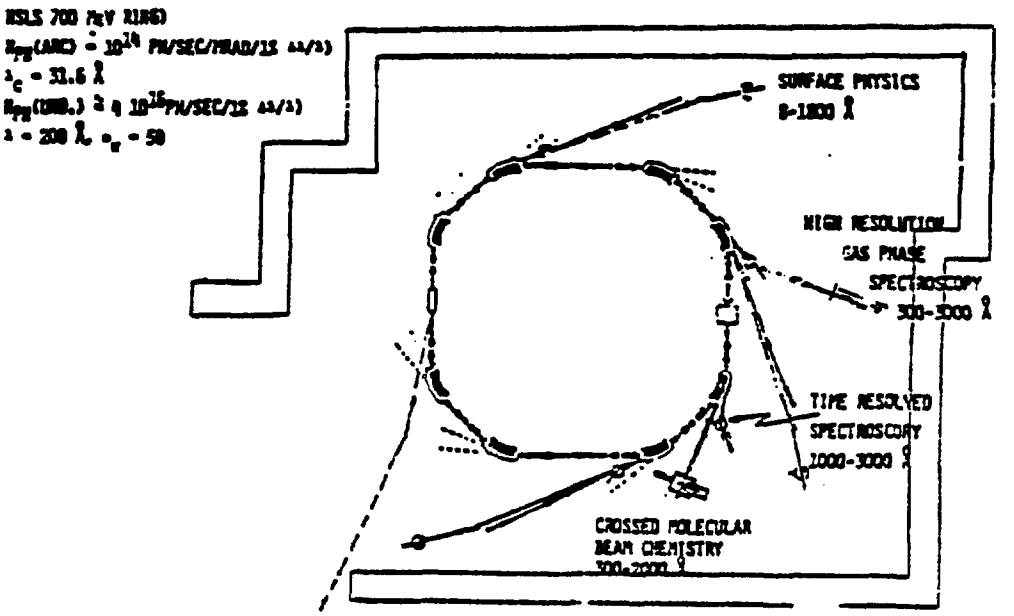

FIG. 7

SYNCHROTRON RADIATION SOURCE FOR VUV SPECTRUM RANGE

TABLE VI

PLANNED FACILITY BEAM LINES

VUV BEAM LINES

11A:	HIGH RESOL. ABPES. [illegible]	35 - 1800 Å
11B:	RES. RESOL. ABPES. IPS. SEAPS	8 - 1300 Å
12:	RES. RESOL. GAS PHASE SPECTROSCOPY	300 - 3000 Å
13:	RES. RESOL. SPECTROSCOPY PHOTOCHEMISTRY. CROSSED MOLECULAR BEAMS	300 - 3000 Å
14:	FLUORESCENT LIFE TIME	- 1200 Å
15:	LITHOGRAPHY. X-RAY MICROGRAPHY	10 - 200 Å

X-RAY BEAM LINES

21A:	SMALL ANGLE SCATTERING. BIOLOGY	0.7 - 4 Å
21B:	SMALL ANGLE SCATTERING. MATERIALS	0.7 - 4 Å
22:	EXAFS. SEXAFS. IPS —0.5 - 4 —4 - 25	0.5 - 25 Å
23:	X-RAY DIFFRACTION CRYSTALLOGRAPHY. DIFFUSE SCATTERING	0.4 - 4 Å
24:	TOPOGRAPHY. DISP. POWDER DIFFRACTION	WHITE BEAM
25/1:	WIGGLER PORT, λ_c = 0.5 Å, λ ≲ 0.1 Å (≲ 100 keV)	

TABLE VII

NATIONAL SYNCHROTRON LIGHT SOURCE

CONSTRUCTION SCHEDULE

FUNDING. PROJECT ORGANIZATION	OCTOBER 1. 1977	✓
ACCELERATED e⁻'s IN LINAC	APRIL 13. 1978	✓
BLDG., CONVENT. FACIL., PRELIM. DESIGN	APRIL 17. 1978	✓
CONTRACT. FOUNDATION & STEEL	SEPTEMBER 20. 1978	✓
"GROUND BREAKING"	SEPTEMBER 29. 1978	✓
CONTRACT. BUILDING	MARCH 8. 1979	✓
BENEFICIAL OCCUPANCY. VUV AREA	[illegible] AUG . 1979	
BUILDING COMPLETE	MAY . 1980	
VUV RING (+ LINAC) (+ BOOSTER)	JANUARY . 1981	
VUV RING. START RESEARCH PROGRAM	JULY . 1981	
X-RAY RING. START RESEARCH PROGRAM	OCTOBER . 1981	

Since a total of approximately 28 beam ports for the X-ray ring and 16 ports for the VUV ring will be used eventually, standardization of the photon line elements between storage ring and external photon line proper will be an objective. This photon line front end[8], of which the basic design is completed, will incorporate all metal slow and protective fast valves, water-cooled collimators and protective shutters, slit assemblies, etc.

In order to facilitate more users than can be accommodated with the initial eight planned monochromatized photon lines, a policy of experimental utilization has been developed for the NSLS, whereby in addition to those beam lines constructed by the NSLS staff for general usage, a number of beam lines would be designed and instrumented by "Participating Research Teams" (PRT's), which, in return, would be given priority for a fraction of scheduled beam time for a specific period of time. In response to a solicitation of interest for future utilization of the NSLS, a substantial number of PRT's are now in formation and are expected to enhance significantly the early experimental utilization of the NSLS.

Status of the NSLS Project

The construction of the NSLS project commenced October 1977 and is planned to be completed by October of 1981. With the possibility of earlier occupancy of the VUV domain of the total building, major emphasis of machine component construction has been on the VUV storage ring. By year end it is expected to test the vacuum integrity of the VUV ring, and with partial excitation, test turn-on capability, from the central control computer via microprocessor links, of the VUV magnet system. Procurement of the rf systems for both storage rings is well advanced, with completion of the VUV rf drive system also being scheduled for October of this year. The 100 MeV linear accelerator injector is presently being commissioned in a temporary location.

It will be moved into the final building, together with the booster synchrotron, during May of 1980. First electron acceleration in the injector complex and storage in the VUV ring is planned for January 1981. Further details of the construction schedule are listed in Table VII.

The start of (partial) NSLS operation is scheduled for July of 1981, with the start of the experimental research program around the VUV storage ring. Similarly, the start of the X-ray ring research program is scheduled for October 1981.

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(7) J. Hastings and W. Thomlinson: "Preliminary Design of the NSLS X-ray Beam Lines", NSLS-BNL Informal Report (in press), May 1979.

(8) J.B. Godel, *et al.*: "Front Ends for the NSLS Experimental Beam Lines", NSLS-BNL Informal Report 26136, May 1979.

NSLS UV BEAM LINES

			λ(Å)	
U 1.	NSLS Diagnostics			
U 2.	-			
U 3.	-			
U 4.	Bell Labs (Rowe, Smith)	A) SEXAFS	12-1200	PGM
		B) ARUPS	80- 500	TGM
		C) REFL/MOD. SPECT.	400-6000	NIM
		D) LITHOG.	White	
U 5.	NSLS Free Electron Laser			
U 6.	IBM (Grobman)	LITHOGRAPHY	White	
U 7.	BNL/SUNY/Penn/Xerox	A) ARUPS/XPS/SEXAFS	15-1200	PGM
	(Strongin, Perlman)	B) ARUPS	80-2500	TGM
	(Jona, Plummer)	C) INFRARED	10^4- 10^6	NIM
U 8.	IBM (Eastman, Spiller)	A) ARUPS	18-2000	TGM
		B) ARUPS	80-2500	TGM
		C) EXAFS/SEXAFS/MICR'Y.	8- 100	Fresnel Zone Plate
U 9.	NSLS/BNL-Bio. (Sutherland)	DICHROISM/FLUORESCENCE	1200-300,000	NIM
	NSLS/BNL-Chem. (Weston)	FLUORESCENCE LIFETIME	1050- 12,000	NIM
U10.	-			
U11.	NSLS/BNL-Chem. (Grover)	GAS PHASE SPECTROSCOPY	300-2000	NIM
U12.	-			
U13.	-			
U14.	NSLS (Howells, Ginter)	A) ARUPS/XPS/SEXAFS	15-1200	PGM
		B) ARUPS	80- 500	TGM
		C) UM. SPECTROGRAPH	300-3000	
U15.	NSLS (Howells)	TGM MONOCHROMATOR		
U16.	-			

NSLS X-RAY BEAM LINES

X 1. - X8	-	
X 9.	Johnson Res. Found. (Chance)	A) EXAFS (Biology) B) Scattering
X10.	Exxon (Cramer)	A) EXAFS B) X-Ray Spectroscopy
X11.	NC State/Conn./BNL (Sayers, Budnick, Pick)	EXAFS
X12.	NSLS/BNL-Bio. (Schoenborn)	A) Small Angle Scattering B) Protein Crystallography
X13.	NSLS/BNL-Chem. (Koetzle, Thomlinson)	Crystallography/Diffuse Scattering
	NSLS/BNL-Physics/Penn/SUNY (Cox, Egami, Prewitt)	Energy Dispersive Diffraction
X14.	ORNL (Sparks)	A) Diffuse Scattering B) Microprobe C) Topography
X15.	Bell Labs	A) Scattering
X16.	Bell Labs (Eisenberger, Golovchenko, Kincaid, Citrin, Moncton)	B) Interferometry C) EXAFS/Scattering D) Spectroscopy
X17.	SUNY (Coppens)	Scattering
X18.	Purdue/Midwest (Liedl)	Diffraction
X19.	NSLS (Hastings)	EXAFS/SEXAFS/XPS
	NSLS/SUNY (Bilello)	Topography
X20.	IBM/MIT (Horn, Birgeneau)	A) Scattering (Low Q Resolution) B) Scattering (High Q Resolution)
X21.	(Reserved for Wiggler)	
X22.	BNL Physics (Shirane)	A) Scattering (High Q Resolution) B) Scattering (High E Resolution)
X23.	NRL/NBS	A) Topography
X24.	NRL/NBS (Kabler, Nagel; Madden, Kuriyama)	B) SAXS C) EXAFS/SEXAFS D) Crystallography E) XPS/UPS
X25.	Wiggler Test	
X26.	Diagnostics	

<u>Unassigned:</u> BNL (Gordon) Microprobe; BNL (Jones) Atomic Physics

AN APPARATUS FOR GAS PHASE STUDIES AT $\lambda \geq 300$ Å

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We are constructing apparatus designed to achieve four criteria:

1) a working region of wavelengths from 300 Å to 2000 Å;

2) absence of all orders higher than the first;

3) intensities as high as possible;

4) able to deal with a significant gas load in the experimental chamber.

In exchange for high intensity and excellent order sorting we are willing to accept only modest resolution, and to forego wavelengths shorter than 300 Å.

The monochromator for this line has already been described by Dr. Howells elsewhere in this report. It is the monochromator he designates U3. A sketch of its layout and a list of its specifications are given in his presentation.

The investigators who are sufficiently interested in this apparatus to commit themselves to membership in the Participating Research Team (PRT) sponsoring it are listed in Table 1.

Table 1

MEMBERS OF PARTICIPATING RESEARCH TEAM

Professor T. Baer, University of North Carolina (Chapel Hill)

Dr. J. Berkowitz, Argonne National Laboratory

Professor W. A. Chupka, Yale University

Professor J. M. Farrar, University of Rochester

Dr. J. R. Grover (Principal Spokesman), Chemistry, Brookhaven National Laboratory

Dr. K. W. Jones, Physics, Brookhaven National Laboratory

Dr. R. B. Klemm, DEE, Brookhaven National Laboratory

Dr. M. O. Krause, Oak Ridge National Laboratory

Professor C-Y. Ng, University of Iowa

Dr. D. J. Seery, United Technology Research Center

Dr. T. Tanzawa, DEE, Brookhaven National Laboratory

Dr. M. G. White, Chemistry, Brookhaven National Laboratory

The members are drawn from a broad spectrum of institutions, including Universities, Industry and the National Labs, and are proposing a wide array of projects, as shown in Table 2. Note that some types of experiments have attracted the interest of several scientists.

Table 2

NSLS/VUV-U3 WINDOWLESS GAS PHASE BEAM LINE: SCIENTIFIC PROGRAMS

TECHNIQUE		EXPERIMENTS	ACTIVE PRT PARTICIPANTS
PHOTOIONIZATION MASS SPECTROMETRY OF MOLECULAR BEAMS	a.	relative photoionization efficiency (fragmentation, autoionization, thresholds)	Baer, Chupka, Farrar, Grover, White
	b.	radicals and reactive molecules	Grover
	c.	analysis of flames	Klemm
	d.	clusters	Gaffney, Grover, White
	e.	ion-molecule reactions	Berkowitz, Chupka Farrar, Ng
COINCIDENCE EXPERIMENTS	a.	Threshold photoelectron/ photoion coincidence (γ, ion/e^-)	Baer, Berkowitz Chupka, Grover, Ng, White
	b.	Ion state selected fluorescence; photoelectron/ photon coincidence (γ, e^-/γ')	Baer

Table 2 (continued)

PHOTOELECTRON SPECTROSCOPY	a.	Angular Distributions	Baer, Krause, White
	b.	Partial Cross Sections	Baer, Krause, White
	c.	Atomic ions	Jones
FLUORESCENCE	a.	Photodissociation of neutrals	Farrar
	b.	Ionic state fluorescence	Baer, Chupka, Farrar, Grover, White
	c.	Lifetimes, dynamics	White
	d.	Matrix isolation	Chupka

Accomodation of such a wide variety of endeavors in one chamber is obviously not feasible. Therefore we have adopted a modular approach. A number of components are supplied, which each worker is free to incorporate into his experiment when his scheduled time arrives. These components are listed in Table 3. All components possess standard flanges for interfacing.

Table 3

UTILITIES LIST

COMPONENT	QUANTITY	REMARKS
General Purpose Collision Chamber	1	Has ten access ports.
500 ℓs^{-1} turbomolecular pumps	2	One pump is part of the nozzle beam apparatus.
270 ℓs^{-1} turbomolecular pump	1	
cryopumps (4-watt closed cycle helium refrigerators)	2	
supersonic nozzle beam apparatus	1	Interchangeable nozzles, helium seeding capability, includes beam dump.
monochromator exit slit assembly	1	Differentially pumped, fast-closing shutter (~5 msec).

Table 3 (continued)

computer + CAMAC	1	Used for monochromator control, but can also be used for data collection
Quadrupole mass spectrometer system, 1-350 AMU.	1	Time-of-flight mass spectrometer will be included later.
Electron spectrometer	1	
Electronics for fast counting, and for coincidence circuits	1	

Thus, each investigator needs to bring only the chambers, etc., that are tailored to his special requirements, taking care to see that he can interface properly with the existing pumps, various instruments, computer, etc. that are already provided.

The configurations for our own experimental program (M. G. White and J. R. Grover) is shown schematically in Fig. 1. Our aim is to cross a molecular beam with the VUV beam (the axis of the photon beam is perpendicular to the plane of the paper), and to detect mass-analyzed ions. The ionizer region is surrounded as completely as practicable with cold walls of ~12 K to minimize background, and to minimize the partial pressure of condensible molecules in the vicinity of the

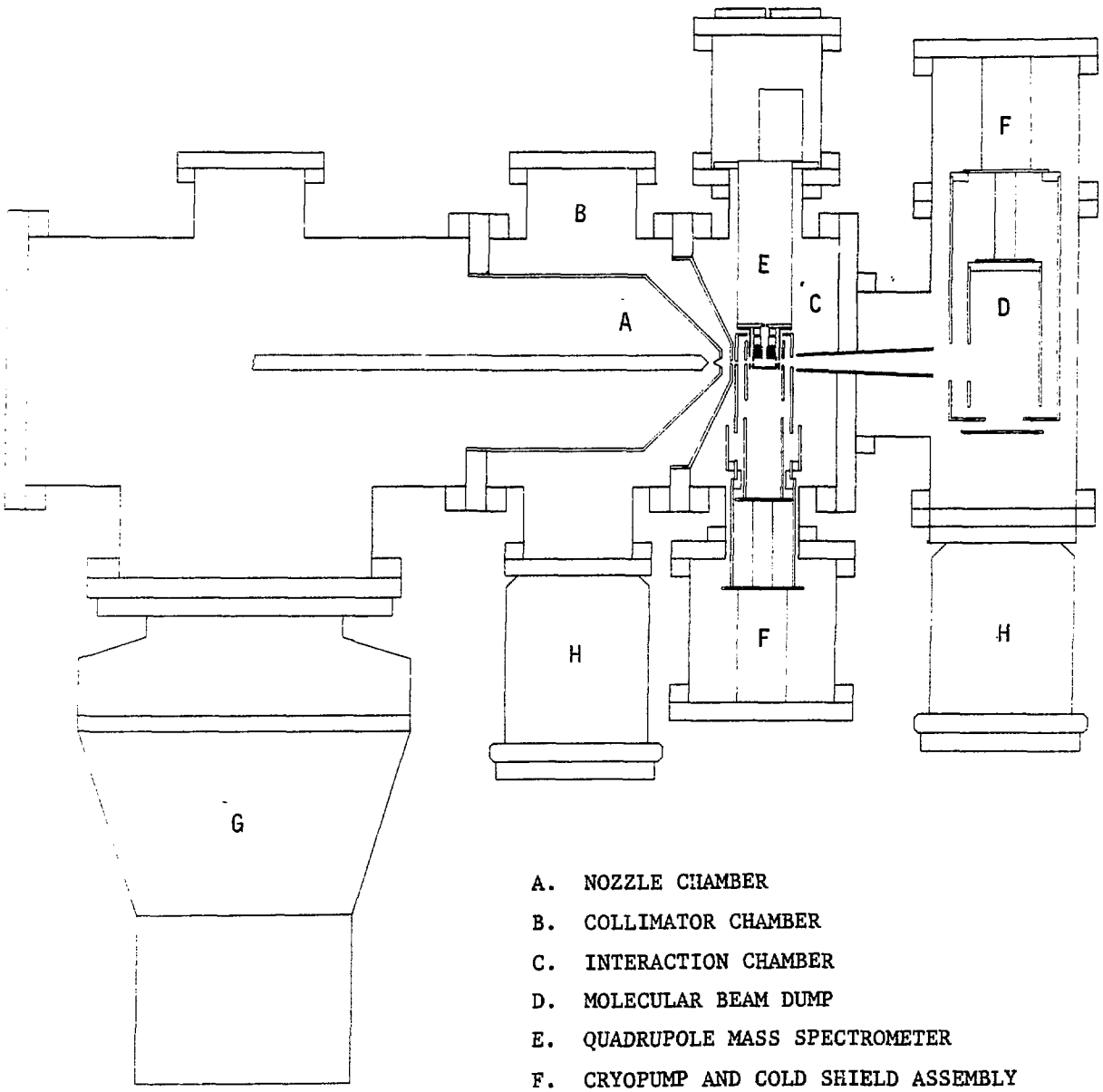
monochromator exit slit. With this arrangement we wish to examine the photoionization excitation functions of some of the many interesting and exotic species that can be made in molecular beams. The large diffusion pump is the only practical way to allow the use of helium carrier gas for seeded beams. To minimize the risk of damage to the monochromator grating and mirror Fomblin oil is used as the pumping fluid, and there are two stages of extremely efficient differential pumping between the diffusion pump and the monochromator line.

Simple reconfigurations of this apparatus will involve interchanging the quadrupole mass spectrometer with a time-of-flight spectrometer to examine cluster-ions of mass larger than 350, and installation of a small electron spectrometer. The latter will allow experiments with threshold electrons to complement the photoionization excitation functions, and also photoelectron-photoion coincidence work in favorable cases. Later we plan to include photoelectron spectrometry and the measurement of photoelectron angular distributions.

We plan first to investigate clusters of hydrogen-bonding molecules, and of metal atoms. Both of these areas command widespread interest among chemists, on both theoretical and practical grounds, e.g. the detailed elucidation of the properties of clusters of Ni atoms would be of great importance. We also plan, at an early stage, to examine free radicals and small, highly reactive molecules, such as CH, C_2, C_2H, NH_2, etc. Most such species have not yet been subjected to VUV experiments, although they are of great interest to chemical theorists because the results are amenable to <u>ab initio</u> calculations, and to chemical kineticists in such fields as combustion and atmospheric chemistry.

Figure 1

NSLS/VUV-U3 WINDOWLESS GAS PHASE BEAM LINE:
BASIC LAYOUT FOR SUPERSONIC
MOLECULAR BEAM-PHOTOIONIZATION
MASS SPECTROMETRY AT NSLS



A. NOZZLE CHAMBER
B. COLLIMATOR CHAMBER
C. INTERACTION CHAMBER
D. MOLECULAR BEAM DUMP
E. QUADRUPOLE MASS SPECTROMETER
F. CRYOPUMP AND COLD SHIELD ASSEMBLY
G. DIFFUSION PUMP
H. TURBOMOLECULAR PUMP

MULTIPLY CHARGED ION SOURCES FOR PHOTON-ION CROSSED BEAM EXPERIMENTS

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The intense beams of synchrotron radiation which will be available from dedicated storage rings such as the x-ray and VUV rings at the National Synchrotron Light Source allow one to contemplate experimental arrangements which can be used to investigate photon-ion interactions in the x-ray and VUV ranges.

Studies of multiply charged ions of charge greater than two and their interactions with photons are of great interest because of the general lack of experimental information about the properties of ground and highly excited states of such ions and the important role some multiply charged ions play in astrophysical and laboratory plasmas. Experimental arrangements which would allow the use of photons as probes of such systems would be invaluable in these studies and would help stimulate research in a thus far untouched but increasingly important area of atomic physics.

Specific experimental arrangements will depend on the aspects of the interaction being studied, but in general the experiments will be technically difficult and by necessity will involve crossed ion-photon beams with concomitant small interaction rates.

For example, if one considers absorption spectra of multiply charged ions in their ground state, it is obvious that the conventional method

of recording the number of photons transmitted through a sample as a function of incident photon energy will not work in the crossed beam case. Nevertheless, it is possible to obtain absorption spectra by recording the radiations (x-rays or Auger electrons) emitted in the de-excitation of the inner shell vacancy created in photoabsorption as a function of incident photon energy. By detecting either fluorescence photons at energies well separated from the excitation photon energy or charged particles (electrons, ions), very rare events can be observed.

The experimental difficulties involved can be appreciated if one considers the following: given 10^{12} monochromatized photons in a synchrotron radiation beam 2 mm in diameter, and a photoabsorption cross section of 10^{-20} cm^2 (worst case), 10^{10} particles/cm^2 are required in order to generate 100 interactions/sec. An appropriate detector with an absolute efficiency of 1% would then yield 1 detected count/sec. Assuming an ion velocity of 10^7 cm/sec (e.g., a 2 keV Ar ion beam), a 2 cm long ion-photon intereaction length, 5×10^{16} particles/cm^2-sec are required, or 1.6×10^{15} particles/sec in a 2 mm diameter beam. A beam of this intensity would require magnetic confinement to prevent its spreading due to space charge, and would be non-trivial to produce.

The situation can be greatly improved in the soft x-ray or VUV range where typical photon-ion cross sections are in the megabarn range. In this case, charged particle beams containing 10^{13} particles/sec or less are required, well within the range of several types of sources of singly and multiply charged ions developed for accelerators used in nuclear physics research. Some of these are well proven, such as the duoplasmatron,[1] of the Penning ionization discharge (PIG) source,[2] while others

are in various stages of development: e.g., electron cyclotron resonance heated plasma sources,[3] or electron beam ion sources[4] (EBIS).

Continuous beams of singly charged ions in the tens of particle microampere range of most of the elements are not too difficult to obtain. Depending on the element, commercially available duoplasmatron or PIG sources (with end extraction) can be readily utilized. Multiply charged ions present another problem. Of all the sources currently available, the PIG is probably the most proven practical design for producing multiply charged ions. A schematic diagram of a Penning discharge source is shown in figure 1. Electrons emitted from the cathode (either thermally heated or due to ion bombardment) are accelerated through the hollow anode, but are prevented from reaching it by the applied axial magnetic field. They are then reflected by the opposite cathode and oscillate back and forth through the anode, producing ions by successive electron impact. The ions are then extracted from a hole in the cathode or anode, though for higher charge states, anode extraction seems to be more efficient. For details and specific examples of such sources, see the article by Bennet.[5]

The highest charge states are obtained from pulsed cold cathode Penning discharge sources which can yield for the noble gases, (Ar, Kr and Xe) 5×10^{13} to 5×10^{14} particles/sec for charge states ranging from +5 to +1.[6] PIG sources have a number of disadvantageous features however: low duty cycle due to the pulsed nature of the source (typically 5%), a very high rate of cathode erosion (due to arcs) which limits the operating time of the source at high power to 4-10 hours, and a rather high gas load since the sources are typically operated at a

pressure of $\sim 10^{-3}$ torr. Such sources would make it difficult to operate for the extended periods of time necessitated by the expected low count rates and would make direct coupling to the storage ring vacuum a difficult task.

Due to the finite confinement time required to generate multiply charged ions by successive electron impact, sources of ions of charge greater than +2 are pulsed repeatedly at fairly low frequencies and have a duty cycle factor significantly smaller than 1. Given that the yield of multiply charged ions is always less than that of singly charged ions, one concludes that crossed photon-multiply charged ion beam experiments executed in a conventional manner would be very difficult if not impossible.

The low duty cycle of multiply charged ion sources would present no difficulties if the ions could be constrained to move in a repetitive fashion along a well defined path in some form of ion trap or perhaps storage ring. Ion trapping by magnetic and electric fields is possible if the ions are formed inside the trap (see article by D. Church in this report), but it is not obvious that one might be able to inject multiply charged ions into such traps and then contain them.

Containing ions in a storage ring is an intriguing idea[7] that merits further study because of the very interesting experimental opportunities afforded by such a device. Some simple considerations define the size and general characteristics of the required ring. If the orbital period of the ion storage ring is matched to the orbital period of the light source, and the ion bunch is of appropriate length, the ions in the bunch are illuminated by all the monochromatized photons from a

synchrotron radiation pulse. The reaction rate per unit cross section or luminosity L is in this case given by:

$$L = N_i \frac{I_\nu}{A} \text{ cm}^{-2} \text{ sec}^{-1} \tag{1}$$

where N_i is the total number of ions in the bunch, I_ν the number of monochromatized photons/sec and A the interaction area of the two beams (in cm^2).

Matching the ion storage ring and electron storage ring orbital periods may be unrealistic, since even for a small sized ion storage ring of say 100 cm circumference, the kinetic energies of the ions would have to be in the MeV range. For example, an ion of mass 100 would require a kinetic energy of ∿1.5 MeV to circulate in such a ring with the orbital period (∿0.6 μsec) of the x-ray ring at NSLS. At more realistic kinetic energies, of the order of 100 keV or more (corresponding to ∿30 kV on the ion source extractor), the orbital period for an ion of mass 100 is 2.3 μsec or less. In such a ring one would expect an ion bunch size which is some significant fraction of the ring's circumference, and an interaction region which is small compared to both the bunch length and storage ring circumference. In this case the luminosity is given by:

$$L = \frac{l}{C} \frac{N_i I_\nu}{A} \text{ cm}^{-2} \text{ sec}^{-1} \tag{2}$$

where l is the length of the interaction region and C the ion storage ring circumference. Taking l = 10 cm, C = 100 cm, $N_i = 10^9$ ions, $I_\nu = 10^{12}$ photons/sec and $A = 3 \times 10^{-2} cm^2$ (2 mm diameter beam) gives $L = 3.33 \times 10^{21}$ $cm^{-2} sec^{-1}$. For a one megabarn cross section, one gets

3.33×10^3 reactions/sec.

An alternating-gradient, separated function small storage ring using electrostatic elements for focusing and bending of ions is feasible in principle, though, as far as can be ascertained, no mention of such a device let alone a choice of stable lattice has been reported to date in the literature. Assuming that a stable lattice can be found, and no serious beam instabilities will occur, the beam lifetime in such a device will be very strongly influenced by the vacuum inside the chamber housing the ring. Charge transfer between residual gas molecules (mostly hydrogen) and multiply charged ions will limit the lifetime to 10-100 sec (assuming a charge exchange cross section in the 10^{-15} to 10^{-16} cm^2 range and a pressure of 10^{-10} torr). A low emittance source of multiply charged ions which operates in an ultra high vacuum environment will be necessary for injecting ions into the ion storage ring.

Whether or not the ion storage ring or some other method of storing the ions proves to be feasible, an ion source capable of providing singly, doubly and triply ionized beams of sufficient ion intensity which can be readily coupled to the electron storage ring vacuum to carry out say photoabsorption measurements would be highly desirable. An ion source with suitable properties and capable of fulfilling the many requirements of a number of the possible options available is the electron beam ion source. The principle of operation of an EBIS is quite simple and a schematic of such a source is indicated in figure 2. A high current density electron beam (10-1000A/cm^2) is launched along the magnetic axis of a solenoid. The beam ionizes atoms of an element introduced as a gas or vapor into the ionization region, and highly charged ions

are formed by successive ionization by electron impact. The ions are contained radially by the attractive potential well due to the negative space charge of the electron beam. In some versions of the source, axial confinement for some period of time is achieved by an appropriate potential distribution impressed on a series of tubes concentric with the electron beam and magnetic field axes, and the distribution modified appropriately at the moment of extraction. In other versions, ions are extracted continuously and the "confinement time" is limited to the ion transit time through the ionization region. The final charge state distribution obtained depends on the bombarding electron current density available, and for a fixed current density, on the ion containment time. In order to maintain the electron beam's radial trapping ability in the confinement mode, very low pressures, 10^{-9} torr or better, are required in the ionization region to avoid space charge neutralization of the beam by residual background gas.

Several versions of the EBIS have been reported in the literature which range from the simple, continuously extracted Giessen version[8] to the cryogenic solenoid versions at Dubna[4] and Orsay.[9]

If one neglects multiple ionization by electron impact and electron recombination processes, both of which appear to be negligible in the ionization region, the charge state distribtuion from an EBIS can be calculated from a simple balance model which describes the change in the density n_i of ions of charge i by the following system of equations:

$$\frac{dn_o}{dt} = - Q_o n_o$$

$$\frac{dn_1}{dt} = Q_o n_o - Q_1 n_1$$

$$\vdots$$

$$\frac{dn_{\zeta-1}}{dt} = Q_{\zeta-2}\, n_{\zeta-2} - Q_{\zeta-1}\, n_{\zeta-1} \tag{3}$$

$$\frac{dn_\zeta}{dt} = Q_{\zeta-1}\, n_{\zeta-1}$$

where $Q_i = \frac{j\sigma_i}{e}$, j is the electron current density, e the electronic charge and $\sigma_i \equiv \sigma_{i\to i+1}$, the ionization cross section for going from charge state i to i+1 ($i=0,1,\ldots\zeta-1$) and ζ is the highest charge state obtained under given conditions. (The characteristic time τ_i is $\frac{e}{j\sigma_i}$. For a sequence of ionization steps from $i = 0$ to $i = \zeta$, $\tau_\zeta = \frac{e}{j}\sum_{i=0}^{\zeta} \frac{1}{\sigma_{i\to i+1}}$.) The solution of the systems of equations (3)is:

$$\frac{n_i(t)}{N_o} = \sigma_o \cdots \sigma_{i-1} \sum_{j=0}^{i} \frac{e^{-Q_j t}}{\prod_{k=0}^{i}{}' (\sigma_k - \sigma_j)} \tag{4}$$

where the prime on the product sign means that the term k=j is to be excluded, and N_o is the neutral atom density at t=0. Finally,

$$\frac{N_\zeta(t)}{N_o} = 1 - \sum_{i=0}^{\zeta-1} \frac{n_i(t)}{N_o} . \tag{5}$$

To investigate the time variation of the $n_i(t)$'s with incident electron energy and beam current density, the following approximate cross sections σ_i can be used:[10]

$$\sigma_i = \frac{1.6\text{x}10^{-13} \ln\left[E/I_{i\to i-1}\right]}{E\ I_{i\to i+1}} \text{ cm}^2 \tag{6}$$

where E is the bombarding electron energy in eV, and $I_{i\to i+1}$ the ionization potential of the most easily removed electron in going from charge state i to i+1. (For tabulated theoretical values of $I_{i\to i+1}$, see reference 11.)

Figure 3 shows the charge state development as function of containment time for argon for the given (unoptimized) incident electron bombarding energy and current density.

The confinement time necessary to reach the highest charge state of interest places a condition on the vacuum inside the source to avoid the above mentioned space charge neutralization of the electron beam by ionized background gas. In order for the ionized background gas density to be less than the beam electron density, the pressure P has to be less than:

$$P < \frac{1.92\text{x}10^{-10}}{\sigma(\pi a_o)^2\ \tau(\text{sec})\ \sqrt{V_e(\text{kV})}} \text{ torr} \tag{7}$$

where σ is the cross section in units of π(Bohr radius)^2 for single ionization of the background gas by electrons of kinetic energy eV_e, and τ is the confinement time. For $\pi a_o^2 \simeq 1$, $\tau = 2\text{x}10^{-2}$ sec and 5 keV electrons, P has to be less than $2.9\text{x}10^{-9}$ torr.

In order to estimate the maximum number n_q of ions of charge q obtained in a pulse after a containment time τ_q, space charge neutralization of the electron beam due to background gas is assumed to be negligible, and equating the ion density to the electron beam density

gives:

$$n_q = \frac{3.333\text{x}10^9 \; I(\text{amp}) \; l(\text{cm})}{\sqrt{E_e(\text{keV})}} \; \frac{f_q}{\sum_{\zeta=0}^{Q} \zeta f_\zeta}$$

where I is the electron beam current in amperes, E_e the electron energy is keV, l is the length of the ionization region in cm, f_ζ is the fraction of ions of charge ζ and Q is the maximum charge attained. If extraction is short compared to the containment time, the number of pulses per second is $1/\tau_q$ and the number of particles N_q per second is

$$N_q = \frac{n_q}{\tau_q} \quad . \tag{9}$$

For example, for argon the various f_ζ's can be obtained at time τ_ζ from figure 3. Assuming a 40cm long ionization region, a 1 ampere, 5 kV electron beam yields $\sim 6\text{x}10^{12}$ triply ionized argon ions per second if the containment time is one millisecond.

A prototype EBIS to be used in atomic physics experiments has been designed and is under construction at Cornell. Figure 4 shows a schematic of the EBIS. The magnetic field is provided by a conventional solenoid which is 50 cm long, and can generate 4.2 kG. The electron beam is launched into the magnetic field from an external, high perveance ($I/_V 3/2 = 2.1\text{x}10^{-6}$), electron gun. An innovative feature of the source is the use of a distributed sputter-ion pump inside the solenoid to produce the ultra high vacuum required in the ionization region. The overall design is relatively simple and inexpensive, and the source can be used either in the continuously extracted or confined beam mode. The source is designed to provide beams of highly charged C, N and O, and

should deliver of the order of ten particle microamperes of singly and doubly charged noble gas ions.

In summary, experimental investigations of say total photon absorption cross section by singly and doubly charged ions are possible. The basic experimental arrangement would consist of a synchrotron radiation beam from an intense source (such as provided by the x-ray or VUV ring at NSLS) crossed with ion beams produced by commercially available or constructed ion sources. The expected low reaction rates would restrict measurements to total ion, electron or photon yields produced as function of incident photon excitation energy. Such experiments will not be easy, but are technically feasible.

Photon interactions involving multiply charged ions of charge greater than three will require new experimental developments and/or approaches. Among the former one may consider undulators which will greatly enhance the synchrotron radiation spectrum as well as significant improvements in multiply charged ion sources, while new experimental approaches may involve arrangements in which the inherently low duty cycle of such sources is compensated for by trapping or circulating the ions for some length of time. Developments along these lines would stimulate research in a thus far untouched but increasingly important area of atomic physics which in turn would contribute greatly to the understanding of the detailed structure and behavior of multiply ionized ions in the ground and highly excited states.

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Figure Captions

FIGURE 1. Schematic diagram of PIG source. Electrons emitted from one cathode are accelerated towards the circular hollow anode, but prevented from reaching it by an applied axial magnetic field. They are repelled by the second cathode and the cycle is repeated. The electrons oscillating between the two cathodes ionize gas introduced into the hollow cathode region.

FIGURE 2. Schematic diagram of an EBIS source. The main components of the source are shown in (b). An electron beam from a high perveance gun is launched into a solenoidal magnetic field whose profile is shown in (a). Multiply charged ions are formed by successive electron impact ionization of ions trapped radially in the space charge potential of the beam, and axially by a potential distribution, solid line in (c), applied to axial beam trap electrodes concentric with the electron beam. To extract the ions, the axial potential distribution is modified, dashed curve in (c). The beam collector collects the electron beam continuously.

FIGURE 3. Time evolution of the fractional ion charge density $N_i(t)/N_o$ in an EBIS assuming negligible multiple ionization by electron impact and negligible electron ion recombination loss.

FIGURE 4. Schematic drawing of the Cornell EBIS. For clarity, gas handling systems and other pumps, valves, etc., are now shown. An innovative feature of this design is the use of a distributed sputter-ion pump to generate the ultra-high vacuum required in the ionization region.

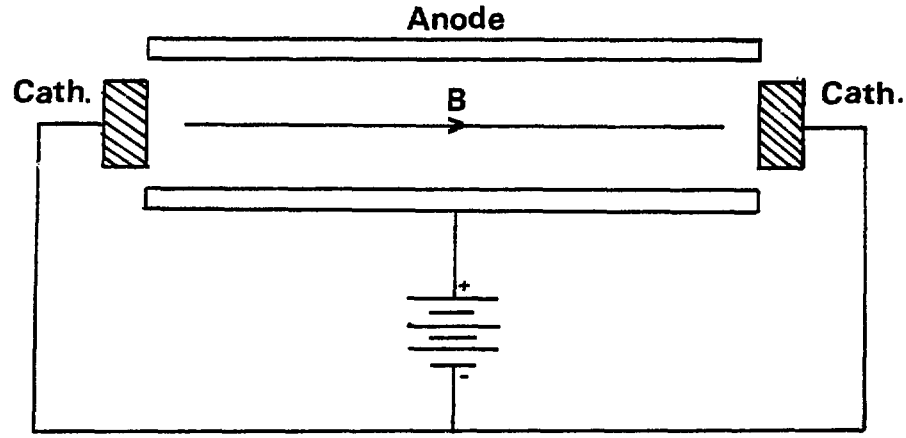
Anode
Cath.
B
Cath.
+
-

FIG.1

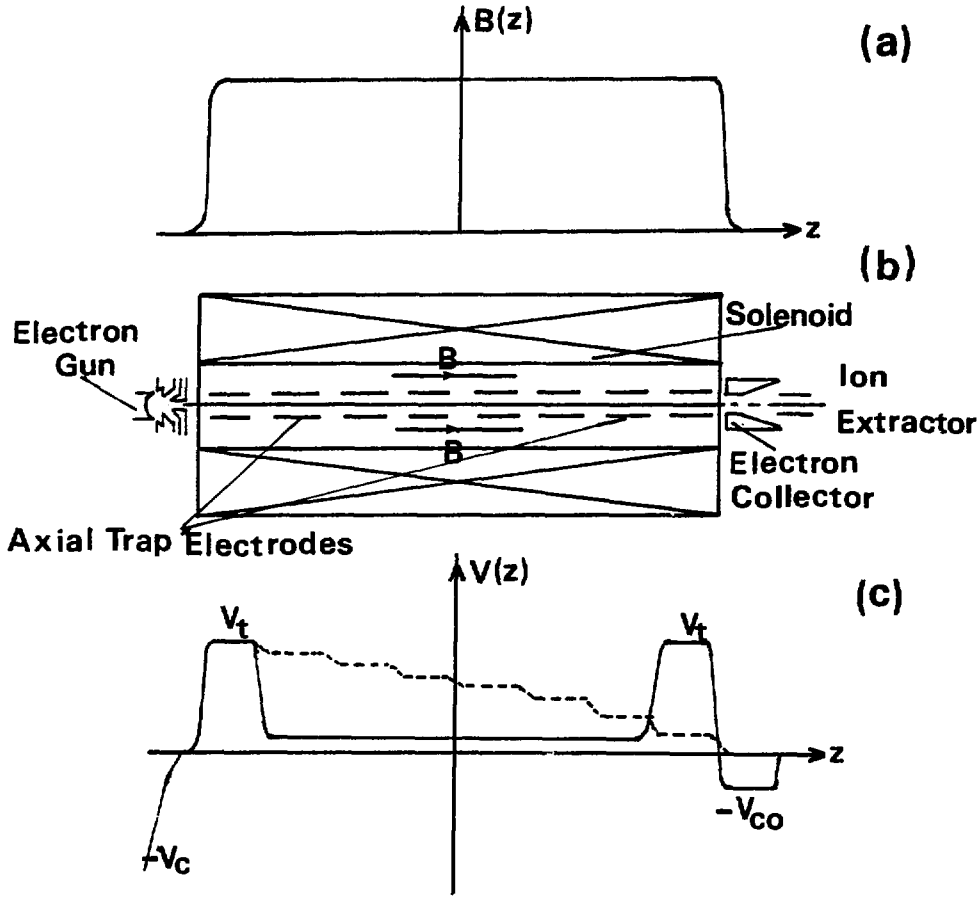
B(z)
(a)
z
(b)
Electron
Gun
Solenoid
B
Ion
Extractor
B
Electron
Collector
Axial Trap Electrodes
V(z)
(c)
V_t
V_t
z
$-V_{co}$
$-V_c$

FIG. 2

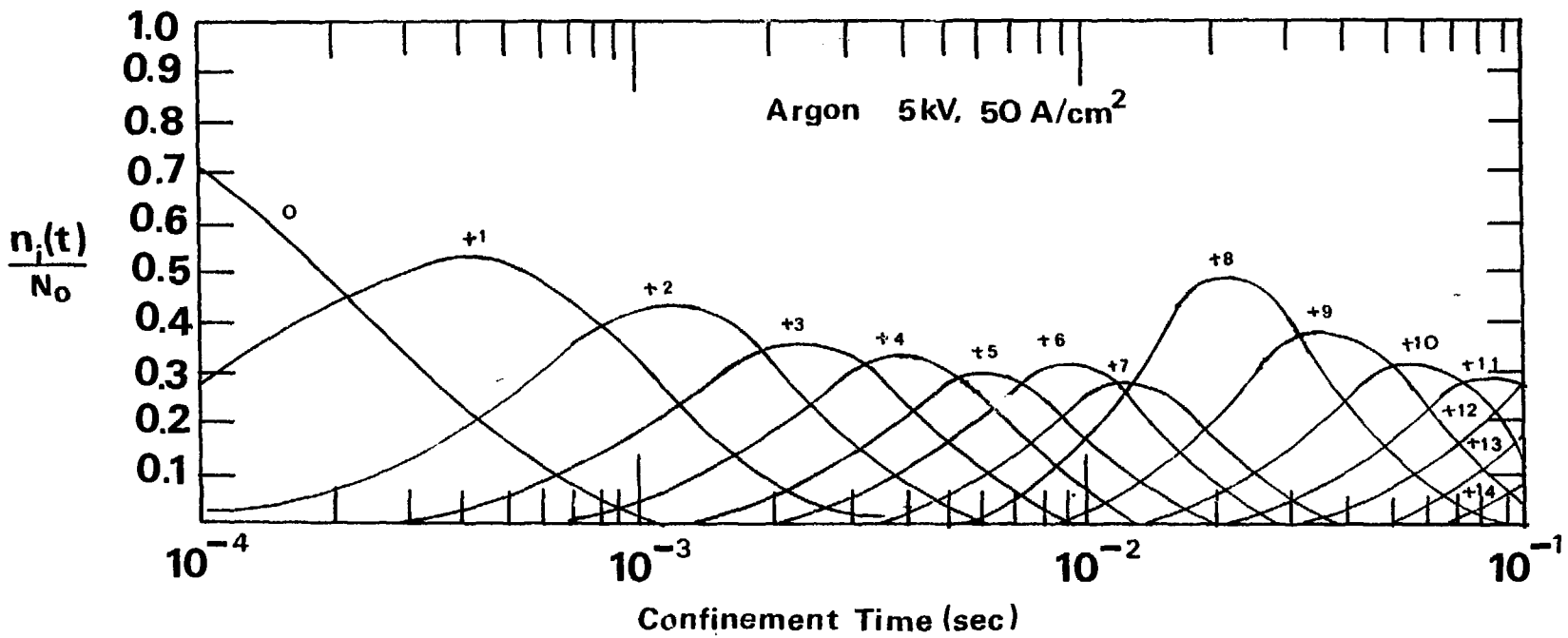
Argon 5kV, 50 A/cm²
$\frac{n_i(t)}{N_o}$
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
+1
+2
+3
+4
+5
+6
+7
+8
+9
+10
+11
+12
+13
+14
10^{-4}
10^{-3}
10^{-2}
10^{-1}
Confinement Time (sec)

FIG.3

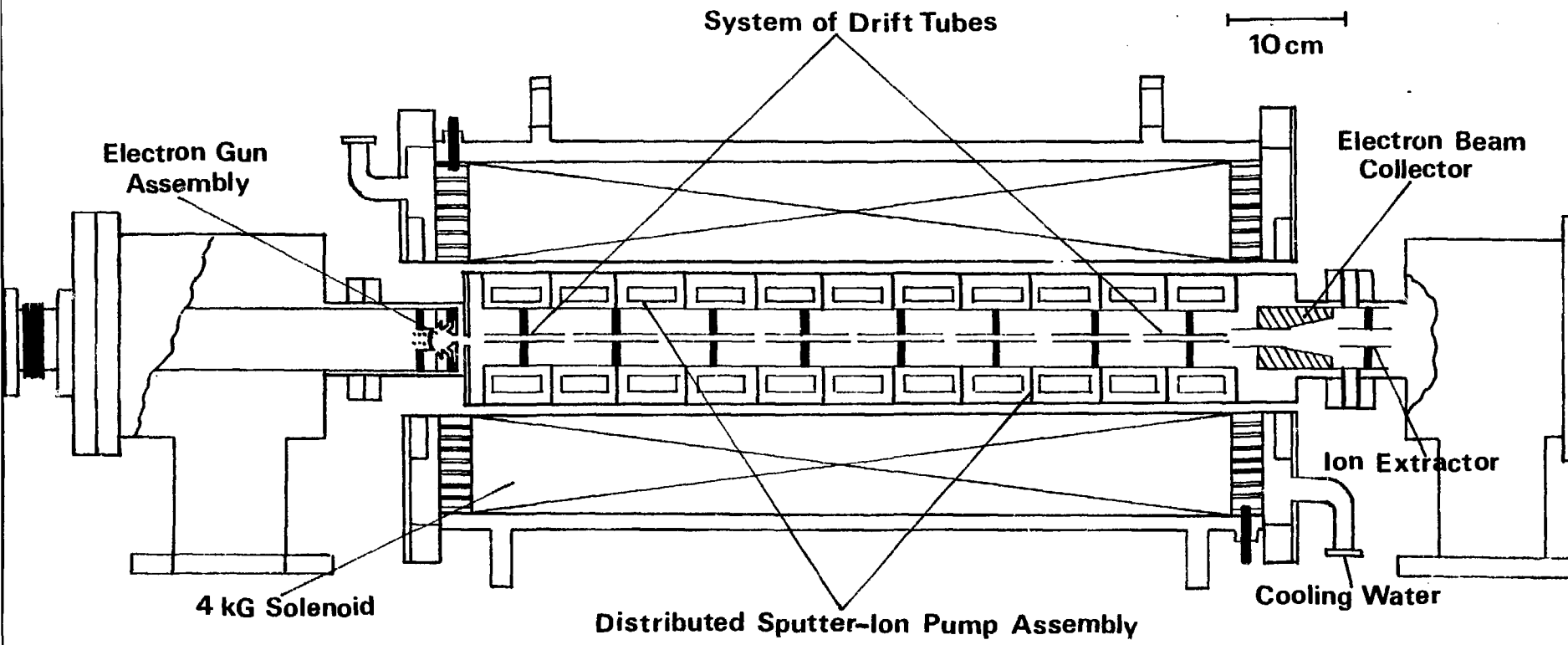
System of Drift Tubes
10 cm
Electron Gun Assembly
Electron Beam Collector
Ion Extractor
4 kG Solenoid
Distributed Sputter-Ion Pump Assembly
Cooling Water

FIG. 4

CONSTRAINTS ON ION BEAM HANDLING FOR INTERSECTING BEAM EXPERIMENTS

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The intense synchrotron radiation beams from the NSLS UV or X-ray storage rings still do not compare in monochromatized photon flux with a laser beam, a fact which becomes apparent in considering reaction rates for interaction of photon and ion beams. There are two prototypical interaction geometries, parallel and perpendicular.

Calculations should properly be done in the rest frame of the ion beam; however, expected beta values are small, so the lab frame will be employed and aberration and Doppler shift effects neglected. For illustrative purposes, particle parameters used will be M = 100amu, K = 10 kev, ($\beta = 4.47 \times 10^{-4}$), σ = 10 megabarns, $i_1/qe = 6 \times 10^{10} sec^{-1}$, and photon parameters $i_2 = 10^{12}$ monochromatized photons per second in an inflexible 2 mm x 2 mm beam.

The particle density in the ion beam is

$$\rho = i_1/qevhw$$

and the reaction signal rate (photon induced)

$$S = \sigma\rho i_2 \times \text{overlap length} ,$$

(w for perpendicular geometry, L for parallel.) The relative rates (parallel to perpendicular) are then L/w, for

same v, where w is the inflexible 2 mm, and it is assumed initially that the two beams have the same, uniform cross section. (Reducing the size of one beam beyond that of the other does not increase the signal rate.) More fully,

$$S_a = \frac{\sigma i_1 i_2 L}{qevwh} ,$$

$$S_b = \frac{\sigma i_1 i_2}{qevh} .$$

The question now arises: are there limits on L (w and h being fixed by the photon beam), leaving for the moment possible variation of v? There are two, in principle: finite source emittance, and space charge blow-up.

In one dimension perpendicular to the z beam direction, using the reasonable, uniformly filled elliptical phase space description in the two coordinates y and y' (= dy/dz), the size of the beam at distance D from a waist (erect ellipse) is given by

$$\hat{y} = \sqrt{\sigma_y^{\,2} + \sigma_{y'}^{\,2} D^2} .$$

σ_y and $\sigma_{y'}$ are not independent, but are related by

$$\sigma_y \sigma_{y'} = E_y ,$$

where E_y is the source emittance (e.g., mm-radians), giving rise to a maximum in D for particular $\hat{y}$ (= 1/2 photon beam size):

$$D_{max} = L_{max}/2 = \hat{y}_m^2/2E .$$

Transverse and longitudinal phase space can be interchanged

by acceleration or deceleration, with conservation of the six dimensional product, the variation in one transverse dimension being as $1/K^{1/2}$. For the Danfysik 911A, assuming $E_y \approx 0.018$ mm-rad, $L_{max} \approx 55$ mm, the relative rates for the two geometries are 55/2 = 27.5. The absolute rates are about $S_a = 6.9$ and $S_b = 0.25\ sec^{-1}$, respectively.

Note that since E_y varies as $K^{-1/2}$ or 1/v, deceleration (in the parallel) case reduces L_{max} to just cancel the 1/v gain in the basic signal rate. Thus, for same v, the parallel case seems to have a decisive advantage. Can v be reduced for the perpendicular case?

Yes, but not without limit. Field-free space charge current limits, which must be considered in both cases, can be estimated from

$$i_1\ (s.c.\ell) \approx 2 \times 10^{-6}\ (v^3/M)^{1/2}(r_o/\ell)^2 \text{ amperes,}$$

[V(ev), M(amu), r_o(beam waist), ℓ(length of travel)]. For example, for 100 amu, $r_o = \frac{1}{\sqrt{2}}$ mm, and ℓ = 50 mm, we obtain

10 kev, i_1 (s.c.ℓ) = 40 microamperes,

1 kev, 1.25 microamperes

100 ev, 40 nanoamperes.

To obtain, in the perpendicular case, the 6.9 counts/second calculated above for the parallel case (10 kev, 10 "particle-nanoamperes"), it would be necessary to slow the beam velocity down by 27.5, decreasing the energy by (27.5^2) to 13.2 ev; then, for ℓ = 2 mm,

i_1 (s.c.ℓ) ≈ 1.2 microamperes .

the ratio of (q+1) to charge q ions might be of the order of a part per billion or less, in the absence of confining schemes such as a solenoid guide field, which might produce a 10x improvement. (Only liquid metal and field emission sources have extremely small emission and very large L_{max}.)

An interesting arrangement for the interaction region would have the character of a three element lens, operated in the accel-decel mode. Looked at from the inside (second element) this involves deceleration in either direction. Depending on the voltages applied it could transmit up-charged ions forward with the parent beam at a different energy, trap the up-charged ions for later release while transmitting the parent beam (both "gates" closed), or reflect the up-charged ions to bend out of the analyzing magnet into a detector on the opposite side from the source (one "gate" closed).

FOR $q' > q$:

GATE 1: $K_1' = q(V_1 + V_2) - q'(V_2 + V_3)$

REFLECTION: $V_3 > \frac{q}{q'} V_1 - \frac{(q'-q)}{q} V_2$

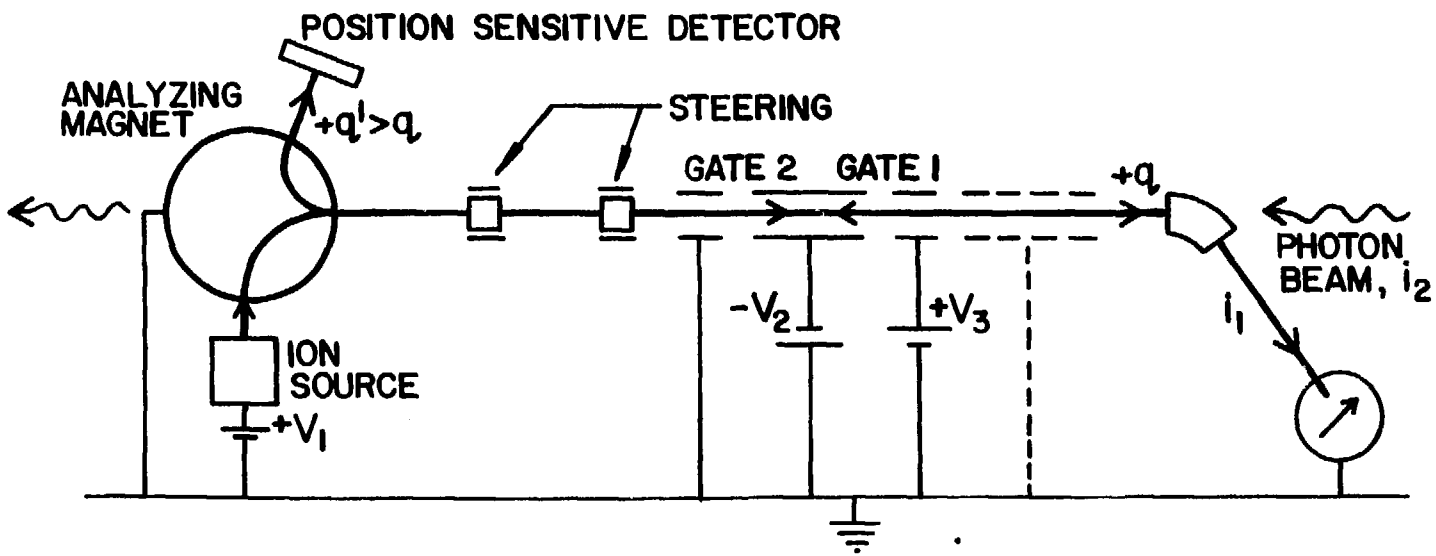
GATE 2: $K_2' = q(V_1 + V_2) - q' V_2$

TRANSMISSION : $V_2 < \frac{q}{(q'-q)} V_1$

FOR q:

GATE 1: $K_1 = q(V_1 - V_3)$

TRANSMISSION : $V_3 < V_1$



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LOW ENERGY ION STORAGE DEVICES

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While high energy physicists have found it expedient to store ions at increasingly higher energies in devices of greater size and complexity, atomic physicists have generally attempted to store ions at ever lower energies, and often in miniturized containers. However, many of the techniques used at both high and low energies are analogous or related.

In atomic physics, ion storage has been predominantly used for precision spectroscopy of long-lived ground[1] or metastable[2] states, where the relatively perturbation-free long-term storage permits narrower linewidths than can otherwise be obtained. The measurement of mean lives of metastable levels of ions[3] holds continuing appeal. Collision measurements take advantage of the long storage times to study processes with small cross-sections, as well as of the controllable low mean energies of the stored ions to investigate the near-thermal or sub-thermal energy regime; examples i clude dissociative recombination[4,5] and ion-atom reactions.[6] Photodetachment of stored, negative ions[7] has also been studied, using a laser as a tunable light source, and photoionization of ions using synchrotron radiation appears to be a realistic possibility.

In all ion storage devices, the maximum ion densities are limited by space-charge effects in $\lesssim$ 10 ev wells to about 10^7 ions/cm^3, which compares well with typical ion beam densities. The ions are typically created by electron impact ionization, although collision reactions are sometimes used. The initially-created energy distribution of the ion gas tends to relax with time toward a thermal distribution characterized by a temperature.[1] The relatively small number of ions usually trapped is compensated by the sensitivity of detection, which can in favorable cases be made as good as a single charge.[8] It is easy to introduce neutral beams of photons or atoms into the trap to prepare particular ion sample states, or to perform chosen collision measurements[1], but charged beams can also be used, e.g. when directed along magnetic field lines, or when the energy of the charges is sufficiently high. The features of weak or controllable perturbations, selectivity of interactions, and confinement of a single identified ion species are significant advantages of the ion storage method. Use of ultra-high vacuum is standard.

Three basic means of ion containment have been used: the dc electrostatic trap, the Penning-type trap with uniform magnetic field and quadrupole dc potential, and the radio-frequency quadrupole trap in either the cylindrically symmetric or storage-ring configurations. Each trapping configuration has characteristic advantages or drawbacks for particular measurements. All of these devices can be built with relatively open structures for photon collection or beam introduction, or with relatively closed electrodes for use as

resonant rf cavities.

1. The Electrostatic Trap (ref 2).

The electrostatic trap has recently been introduced by Prior and Wang[2] to study the hyperfine-structure of the metastable 2 $^2S_{1/2}$ level of $^3He^+$. It has the advantages of no required magnetic field which would decouple the hfs, and no strong rf fields to Stark quench metastable levels. The basic device is shown schematically in Figure 1, and its properties summarized in Table 1. It is based on the ion gauge structure. Ions are produced in the device by ionization of residual gas by axially injected electrons. The ions are conditionally stable, their confinement depending on the maintenance of orbits which do not intersect the central wire. Since the ions do not have characteristic motional frequencies, the mass-to-charge ratio m/q of the stored ions must be identified by characteristic scattering or emission of radiation, or by ejection into a m/q selective device.

TABLE I

Data for Electrostatic Trap (ref 2)

A. Required fields: dc electric, with potentials $V_{dc} < 15$ V.

B. Trap Dimensions: length = 30 cm, active volume = 400 cm^3

C. Ion parameters ($^3He^+$):

ion density = $10^5/cm^3$

ion number = 4×10^7

mean ion energy = 1 eV

storage time near 10^{-8} torr: $\leq$ 0.5 seconds.

D. Characteristic ion motional frequencies: none

E. Detection of specific ion m/q ratios:

ion ejection into rf quadrupole analyzer

resonant laser light scattering

characteristic photon emission

F. Resolution of m/q detection: determined by external detection apparatus.

II. The Penning Trap (ref 9):

The Penning trap, shown schematically in Figure 2, uses a strong uniform external magnetic field for radial containment. This field overcomes the radial defocussing action of the dc potential used for axial confinement. Electrons injected along the magnetic field lines ionize the residual gas. A confined ion moves with axial angular frequency $\omega_z=(qV_0/mZ_0^2)^{\frac{1}{2}}$ in a trap where the cylindrical ring electrode is at potential V_0 with respect to the end cap electrodes separated by a distance $2z_0$. The electrodes are usually machined to the shape of hyperboloids of revolution, and correction electrodes have been sometimes used.[10] The radial motion of the ions has two characteristic frequencies: $\omega_+ = \omega_c/2 + (\frac{\omega_c^2}{4} - \frac{\omega_z^2}{2})^{\frac{1}{2}}$ and $\omega_- = \omega_c/2 - (\frac{\omega_c^2}{4} - \frac{\omega_z^2}{2})^{\frac{1}{2}}$, where $\omega_c = qB/m$ is the cyclotron angular frequency. When $\omega_c \gg \omega_z$, $\omega_+ \approx \omega_c - \omega_-$ and $\omega_- \simeq \frac{\omega_z^2}{2\omega_c}$. Thus the motion is entirely harmonic, and the problem of a single charge moving in the potentials has been solved classically[9] and quantum mechanically.[11] This trap provides excellent m/q identification by cyclotron resonance. The detection of ions by rf spectroscopy, and storage times of hours

or days in ultra high vacuum, are used to advantage whenever the presence of a large magnetic field is not a deterrent. To reduce the mean ion energy to room temperature or below, the stored ions may be cooled stochastically via feedback of ion-induced voltages,[12,13] collisionally with other ions or with atoms,[1] and by resonant scattering of slightly Doppler-shifted laser radiation.[14,15]

TABLE 2

Data for a Penning-type trap

A. Required fields: uniform magnetic ($B \gtrsim 1$ T)

and dc electric (potential $V_0 \lesssim 25$ V).

B. Trap dimensions: axial: $2z_0 \simeq 1.4$ cm, $r_0 = 2^{1/2} z_0$

C. Ion Parameters (N^+)

ion density $\simeq 10^6/cm^3$

ion number $\simeq 10^5$

mean ion energy $\simeq 1$ eV

storage time near 10^{-8} torr: $\simeq 10$ sec.

D. Characteristic ion motional frequencies:

ω_+ = shifted "cyclotron" frequency = $2\pi \times 7$ MHz

ω_z = axial oscillation frequency = $2\pi \times 600$ kHz

ω_- = drift frequency = $2\pi \times 39$ kHz

E. Detection of specific ion m/q ratios:

Rf spectroscopy of ion motional frequencies

ion motion induced currents

resonant ejection into particle multiplier

resonant laser light scattering

F. Resolution of m/q detection:

cyclotron resonance $Q \gtrsim 10^4$ depending on B field homogeniety

axial resonance $Q \approx 150$, depending on electrode configuration

III. The Radio-Frequency Quadrupole Trap (ref 1)

In a device with electrode geometry of the form used in the Penning trap above, see Fig. 2, a potential of the type $\Phi = (V_{dc} - V_{ac} \cos\Omega t) \times \left(\frac{r^2 - 2z^2}{2r_o^2}\right)$

leads to ion motion governed by the Mathieu-type differential equation, written in standardized form $\frac{d^2X}{d\eta^2} + (a-2q \cos 2\eta)\, X = 0$ where $\eta = \frac{\Omega t}{2}$, $a_r = \frac{4qV_{dc}}{m\Omega^2 r_o^2}$, $q_r = \frac{2q\ V_{ac}}{m\Omega^2 r_o^2}$, $a_z = -\ 2a_r$, $q_z = 2q_r$ and X is a generalized coordinate representing x, y or z. If the parameters a_r, a_z and q_r, q_z together simultaneously have values lying in parameter space in the "region of stability", the charge is stably confined; i.e. the amplitude of the motion is bounded. Outside of the stability region, the amplitude of the motion grows exponentially with time.

The ions move with a characteristic frequency spectrum having terms $n\Omega \pm \omega_{r,z}$, n taking on integer values form 0 to ∞, and $\Omega > 2\omega_{r,z}$. However, the amplitudes of terms with $n \gtrsim 2$ decrease rapidly. By the proper choice of parameters, generally made by adjusting the dc and ac potentials, either a large range of ion m/q ratios can be simultaneously trapped, or with another choice, and favorable electrode tolerances the range can be restricted to a single m/q. For many purposes the ions can be visualized as moving in a "pseudo" dc well, with an exchange of energy between large amplitude oscillations

at $\omega_{r,z}$ (kinetic energy) and smaller amplitude vibrations at Ω (potential energy).

Rf quadrupole traps provide many of the features of the Penning trap, with the advantage of no magnetic field if none is desired, or with small adjustable uniform magnetic fields superimposed.[1] The ions can be detected by rf resonance with a Q near 100, lacking the higher resolution available with cyclotron resonance. Other detection means used in Penning traps also apply. The ions can be cooled stochastically,[13] collisionally,[1] and by laser radiation scattering,[16] but there is a small residual heating mechanism,[13] not fully understood, which must be overcome. Massive ions are generally easier to confine for longer times than lighter ones.

TABLE 3

Radio-Frequency Quadrupole Trap (ref 1)

A. Required fields: dc electric, rf electric with a potential V_{RF} = 137 V at $\Omega/2\pi$ = 1 MHz, and which increases as $\Omega^2 r_0^{\ 2}$.

B. Trap diminsions: axial: $2z_0$ = 5 cm; $2r_0$ = 7.2 cm.

C. Ion parameters ($^3He^+$):

ion density $\approx 10^7/cm^3$

ion number $\approx 8 \times 10^6$

mean ion energy $\approx$ 1 eV

storage time near 10^{-8} torr: 8 seconds

D. Characteristic ion motional frequencies

$\omega_z = 2\pi \times 134$ kHz, ω_r generally $\neq \omega_z$

$n\Omega \pm \omega_{z,r}$ (Ω = trapping rf frequency, n = 0,1,2,....)

E. Detection of specific ion m/q ratios:

rf spectroscopy of motional frequencies

ion motion induced currents

resonant ejection into particle multiplier

resonant laser light scattering

characteristic photon emission

F. Resolution of m/q detection:

rf resonance $Q \approx 100$, otherwise determined by external detection apparatus.

IV. Storage ring rf trap:

Storage ring traps[17] are very similar in operation and properties to the rf quadrupole trap, but have a stability diagram of different shape in parameter space, due to the essentially 2-dimensional nature of the confinement. The storage ring is constructed by bending a linear two-dimensional quadrupole into a circular or racetrack shaped structure, see Fig. 3. The ions move freely around the track, but are confined radially. The bends must be small enough to avoid significant perturbation of the ion motion. A ratio of track radius R to quadrupole radius r_0, $R/r_0 \approx 45$ has been found adequate. Nevertheless the perturbation of the ideal structure results in non-confinement or reduced storage times at certain parameter values normally expected to be stable. Difficulty in maintaining dimensional tolerances in the larger ring structure reduce the Q of resonant ion detection to about 20. The

principal advantage of the storage ring lies in the relatively long interaction region available for ion collisions with well-collimated neutral beams.

TABLE 4

Storage Ring RF trap (ref 17)

A. Required fields: Radio-frequency electric; V_{RF} increases proportional to $\Omega^2 r_0^2$, V_{RF} about 200 V at $\Omega/_{2\pi} \approx 52$ MHz

B. Trap dimensions: structure diameter 14 cm, interelectrode diameter $2r_0 = 0.32$ cm.

C. Ion parameters (H^+)

ion density = $10^5/cm^3$

ion number = 10^5

mean ion energy ≈ 0.8 eV

storage time near 10^{-8} torr: ≈ 8 seconds.

D. Characteristic ion motional frequencies

$\omega/_{2\pi} = 4.5$ MHz

$n\Omega \pm \omega$, $n = 0, 1, 2, \ldots$

E. Detection of specific ion m/q ratios:

rf spectroscopy of ion motional frequencies

F. Resolution of m/q detection

rf resonance Q ≈ 20.

Photoionization of Stored Ions:

Studies of photoionization of ions might usefully be performed using a stored ion gas as a target for synchrotron radiation. The customary method of detecting the electrons might appear not to be effective for trapped ions, since the trapping fields will certainly have a profound effect on the trajectories of the much lighter electrons. However, it has been demonstrated that low energy electrons can be extracted from a Penning trap for subsequent energy distribution analysis,[18] and it may be possible to achieve some acceptable degree of energy resolution for photoelectrons as well. In the Penning structure, the electrons are confined along the magnetic field lines after production, and leave the trap through the end electrodes with kinetic energy determined by their production process and by their location at production in the dc potential. A photon beam directed across the magnetic field lines through the center of the trap potential will produce electrons of nearly the same energy in the well, and an interaction region is radially defined by the apertures for the collection of electrons from the trap. Electron angular distribution measurements would not be possible unless some means were found to discriminate motional energy for electrons emitted perpendicular to the magnetic field, from those emitted parallel to it.

Alternatively, the detection of ions produced by the photoionization process would provide a direct means of investigating

final charge states, and provide a possibility of integrating weak ion number signals. Here the photon beam might best be directed along the magnetic field, in the same region where the ions are created, since in ultrahigh vacuum radial diffusion of the charges is slow. With an ion density of $10^7/cm^3$, an interaction region length of 0.5 cm, and a cross-section for photoionization near an absorption peak of 10^{-19} cm^2, a photon flux of 10^{14}/sec produces about 50 ions per second. Since larger photon fluxes are available, and single ion detection by, e.g. resonance ejection into a particle detector, is possible, the method appears feasible.

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Research supported by the Department of Energy, under contract number DOE /5/05-6043, and by the TAMU Center for Energy and Mineral Resources.

A complete bibliography is not given, due to the general review being prepared by G. H. Dunn, D. J. Wineland, and F. L. Walls for publication in Advances in Atomic and Molecular Physics, Vol. 17, to appear shortly. Nevertheless, the articles cited should lead to most of the published work in the field. See particularly ref. 1 and ref.4.

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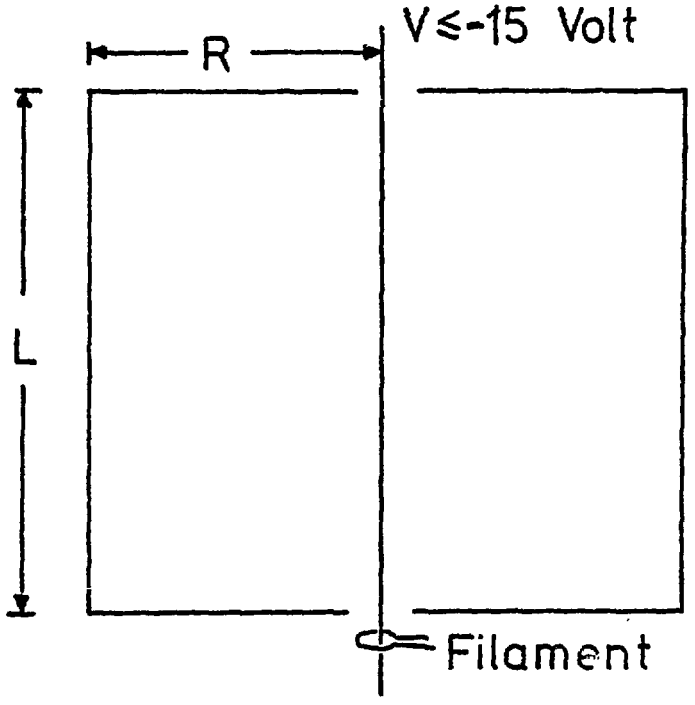

Figure 1. Schematic diagram of electrostatic ion trap

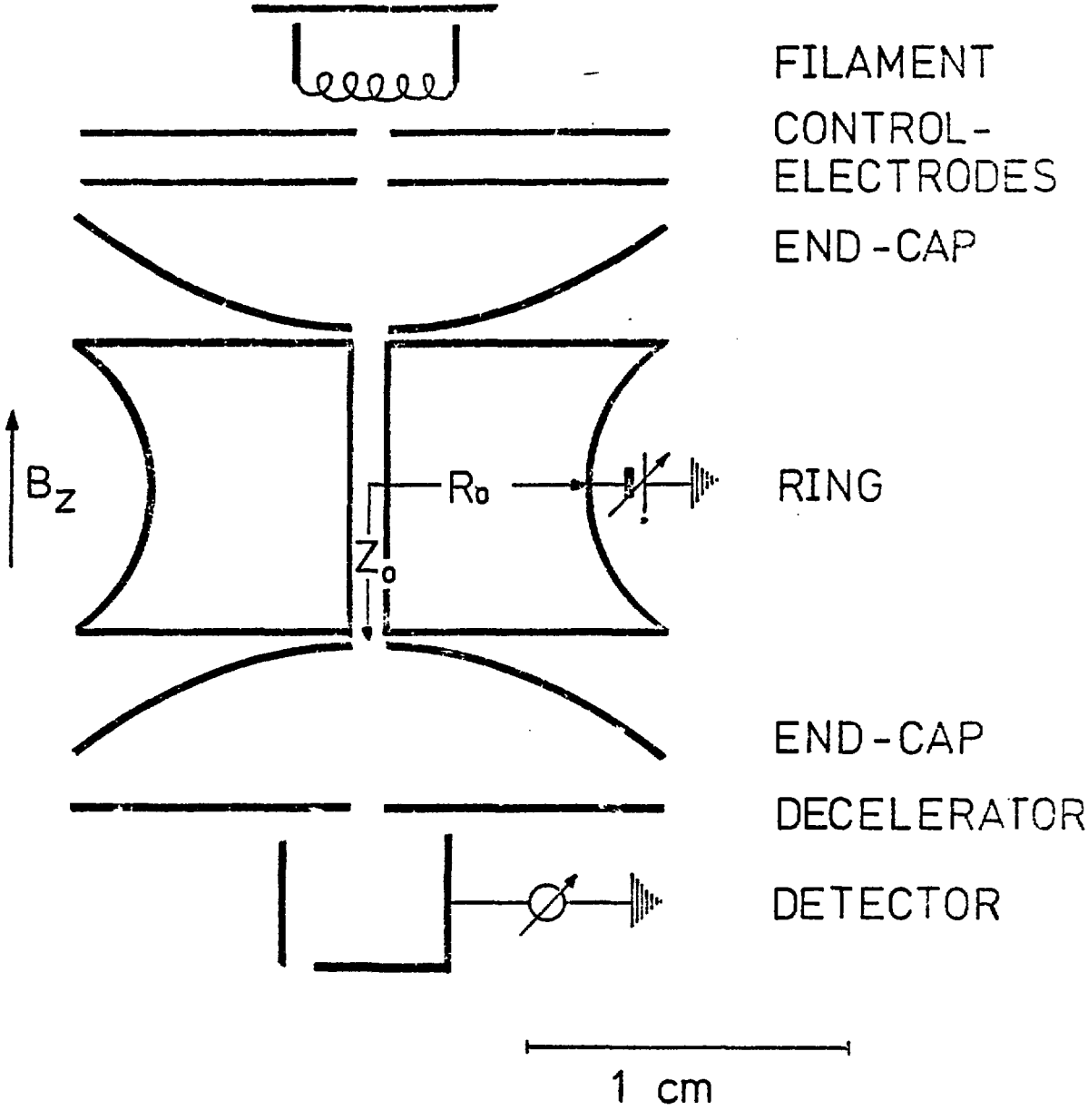

Figure 2. Schematic diagram of quadrupole structure used in the Penning Trap, with axial magnetic field B_z, or the RF quadrupole trap, with B_z=0. Generally $R_o = \sqrt{2}\, Z_o$, and the electrodes are hyperboloids of revolution.

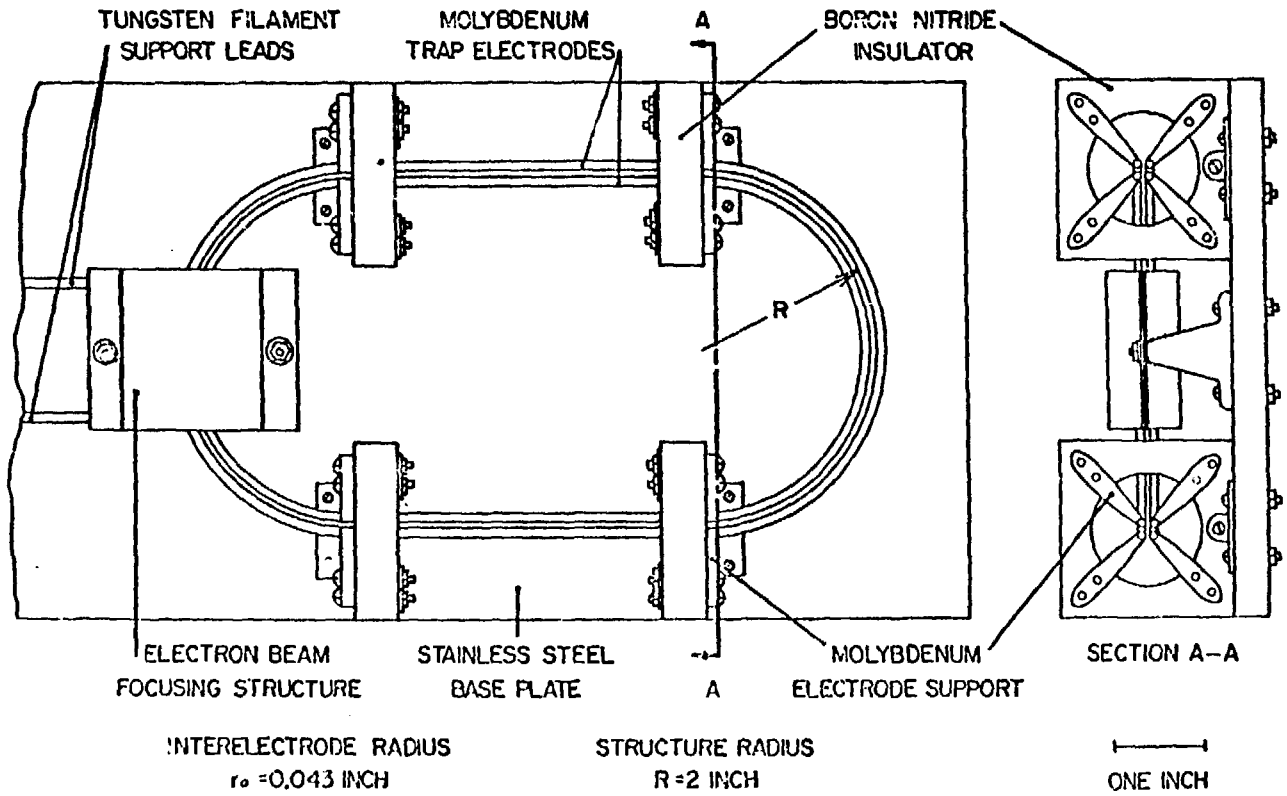

Figure 3. RF quadrupole storage ring ion trap (taken from Ref. 17)

PHOTON DETECTION IN THE VUV

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The fundamental processes involved in the detection of vacuum ultraviolet (VUV) radiation are the photoelectric effect and photoionization of a gas.

Because VUV radiation cannot pass through regular glass windows it is necessary either to convert the energetic VUV radiation to longer wavelengths by the use of scintillators such as sodium salicylate or to use special transparent windows such as LiF, MgF_2, etc. After the VUV or fluorescent radiation has passed through into the detector (typically a conventional photomultiplier) its presence is ususally detected by the photoelectric effect from some suitable photocathode. However, for shorter wavelengths windowless detectors are necessary. Simple photocathodes can still be used by themselves or coupled to an electron multiplying structure. The photocathodes, however, need to be stable on exposure to air when stored for any length of time. When photoionization of a gas is used as a detector system thin windows of plastic or metals about 1000 to 2000 Å can be used to contain the gas depending upon the wavelength region of interest. Alternatively, gases can be used in windowless systems by the use of good differential pumping. Detection of VUV radiation based on these principles has led to the following types of detectors most commonly used in the VUV spectral region (2 -2000 Å).

Photomultipliers:	(a)	with sodium salicylate coating
	(b)	used with LiF, MgF_2, sapphire windows, etc. (EMR type photomultipliers)
Windowless electron multipliers:	(a)	discrete dynodes
	(b)	channeltrons
	(c)	microchannel plates
	(d)	continuous strip magnetic field multipliers
Photodiodes:	(a)	with or without windows
Ion chambers:	(a)	gas fillings are typically the rare gases or nitric oxide
Geiger/Proportional Counters:	(a)	typical gas filling is methane

The above list summarizes the most useful detectors currently in use. Rather than describe each detector separately we will discuss only particular aspects, some of which are not commonly known.

The photoelectric yield of a material is the fundamental quantity that characterizes the response of most photomultipliers and photodiodes. In the windowless region most photocathodes are simple clean metal surfaces or the high resistive surfaces of channeltrons and microchannel plates. However, for either surface the photoelectric yields, as a function of wavelength, are surprisingly similar. Figure 1 shows a typical yield curve for Al. Any metal surface has an absolute yield within $\pm$ 30% of that shown in Fig. 1.[1] The efficiency can be improved by allowing the radiation to impinge at a grazing angle onto the cathode, and still further improvement can be obtained by collecting the lost radiation caused by reflection.[2] Figure 2 illustrates this procedure for several reflections from Al cathodes. The dashed curve is the yield for radiation incident at right angles to the phtotocathode surface. It is important to know the sensitivity of a photo-

cathode as a function of position across the sensitive area. In most photodiodes the sensitivity is relatively constant. However, when a photocathode is used with a multiplying structure the collection efficiency of electrons into the multiplying structure may not be constant. An important example of this is found with the Bendix magnetic multipliers with a continuous strip dynode structure. A typical curve is shown in Fig. 3.

Metal photocathodes are the most generally useful surfaces. They are stable, rugged, and easily cleaned. They have been adopted for use as secondary standards in determing the absolute photon flux in the VUV.[3,4] Figure 4 illustrates the efficiencies of an Al_2O_3 and W photocathode over the range 50-1200 Å. Of course, for some specific uses thin film of LiF, MgF_2, CsI, etc can be evaporated onto the metal photocathode to give yields up to 40 or 60% at certain wavelenghts.[5-6]

The other important method for VUV detection is based on the photoionization of gases. When absolute photon intensities are desired the photoionization method becomes the most important detector. With a properly constructed ion chamber filled with a rare gas the ion chamber detector becomes an absolute standard.[6] Figure 5 shows the cross-section of a typical standard ion chamber.[7] The ion collector plate is split precisely in the middle of the ion chamber. All of the ions in the first half must go to the i_1-plate, whereas the ions in the second half must go to the i_2-plate. Under those conditions the absolute photon flux I is given by

$$I_o = \frac{i_1^2 / e}{i_1 - i_2} \quad \text{photons/sec,}$$

Where e is the electronic charge and the currents i_1 and i_2 are measured in

amperes.

To obtain more sensitivity than is found in a simple ion chamber use can be made of the geiger or proportional counter. Although many descriptions of these devices have appeared in the literature[8] of specific interest is the proportional counter that is new commercially available from the J.E. Manson Co.[9] The counter operates with methane gas in a flow system that maintains a pressure of about 60 Torr for use in the VUV region and about 200-800 Torr for use in the x-ray region. Other gases, of course, could be used. A thin plastic window of VYNS (10% vintl acetate and 90% vinyl chloride) mounted on a high transmission mesh provides an excellent vacuum seal. The detector is essentially 100% efficient after the radiation passes through the window (depending on the pressure of the methane). Thus the detector response is basically that of the window. A transmission curve is shown in Fig. 6 from 2 to 500 Å. Thin film windows made from Al, C, In, etc can also be used provided they are gas tight. This allows other spectral regions to be studied. When the transmission of the window is known the absolute intensity of the radiation can be determined, especially in the x-ray region.

The choice of a detector depends on the nature of the experiment and the sensitivity required. But certainly the sodium salicylate coated photomultipliers and simple photodiodes are the most general detectors of VUV radiation.

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Figure Captions

Fig. 1. Photoelectric yield of aluminum

Fig. 2. Photoelectric yield of aluminum. The dashed line indicates the yield obtained when the radiation is incident at right angles to the surface of the metal. The solid line shows the increased yield obtained when the radiation is incident at an angle of 80^0 with the reflected radiation captured by successive cathodes also at 80^0.

Fig. 3. The absolute efficience of a Bendix multiplier as a function of position along the photocathode. The zero position is nearest to the multipling section.

Fig. 4. Photoelectric yield of an Al_2O_3 and W secondary standard as obtained by NBS (see ref. 3). The efficiencies for other photocathode materials as used by Stanford and EMR are also shown.

Fig. 5. Double ion chamber suitable for absolute intensity measurements.

Fig. 6. Transmission curve for a thin window of VYNS material.

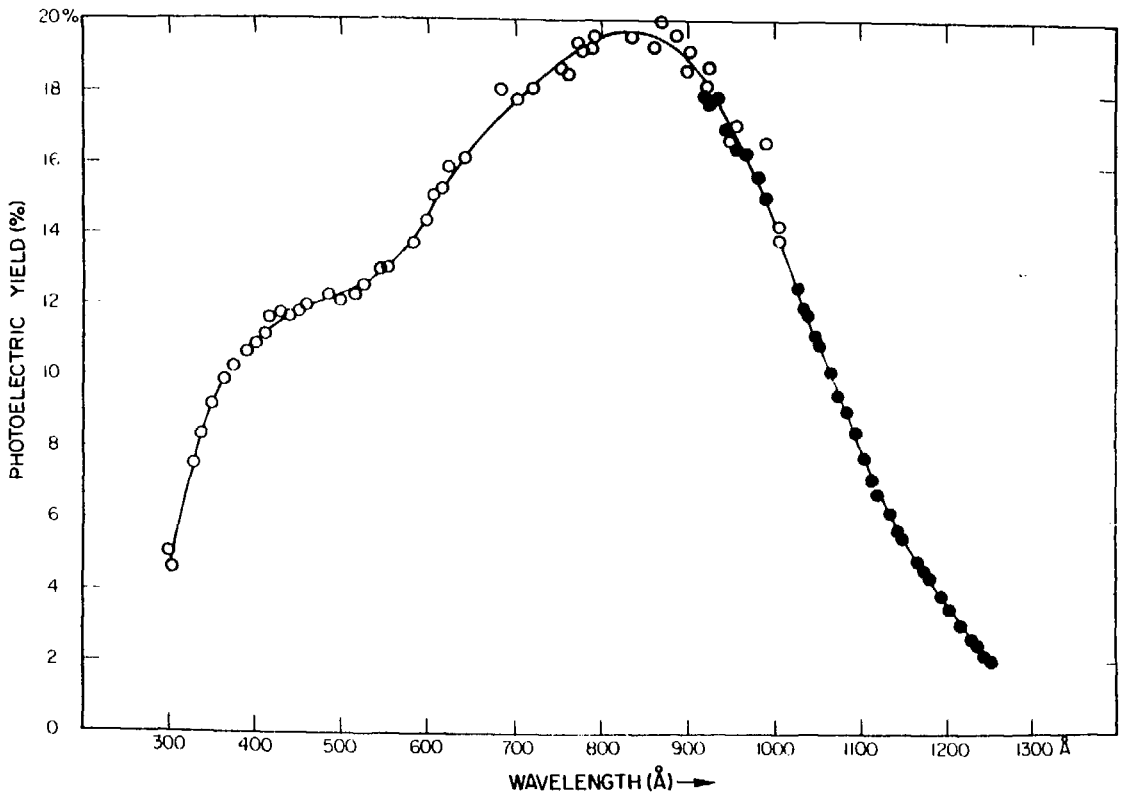
20%
18
16
14
12
10
8
6
4
2
0
PHOTOELECTRIC YIELD (%)
300
400
500
600
700
800
900
1000
1100
1200
1300 Å
WAVELENGTH (Å)

Fig. 1

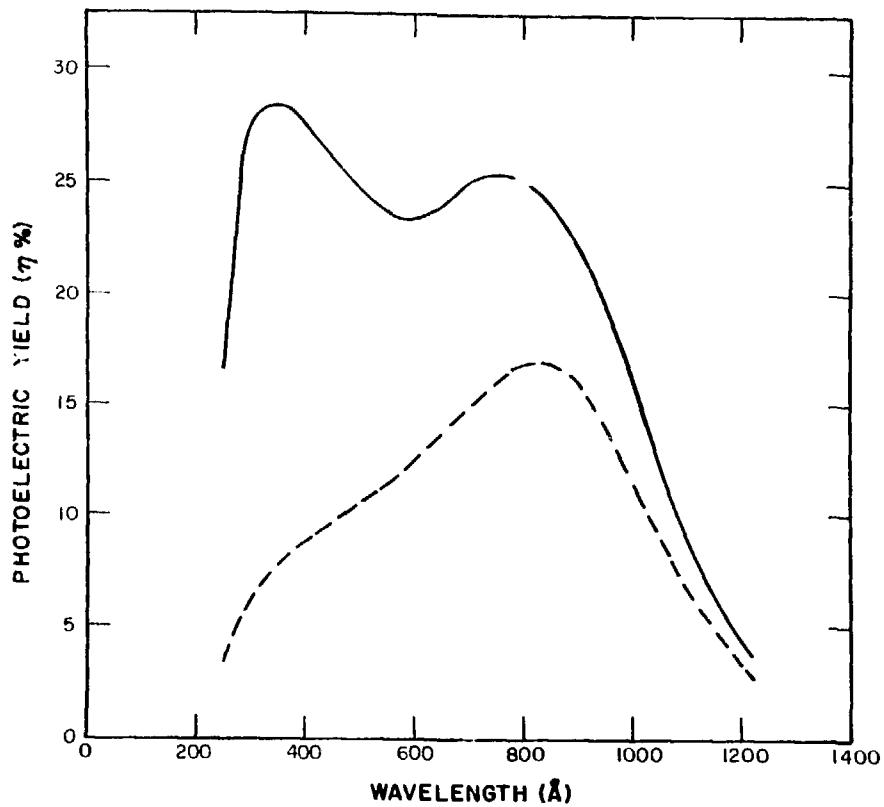
PHOTOELECTRIC YIELD (η %)
30
25
20
15
10
5
0
0
200
400
600
800
1000
1200
1400
WAVELENGTH (Å)

Fig. 2

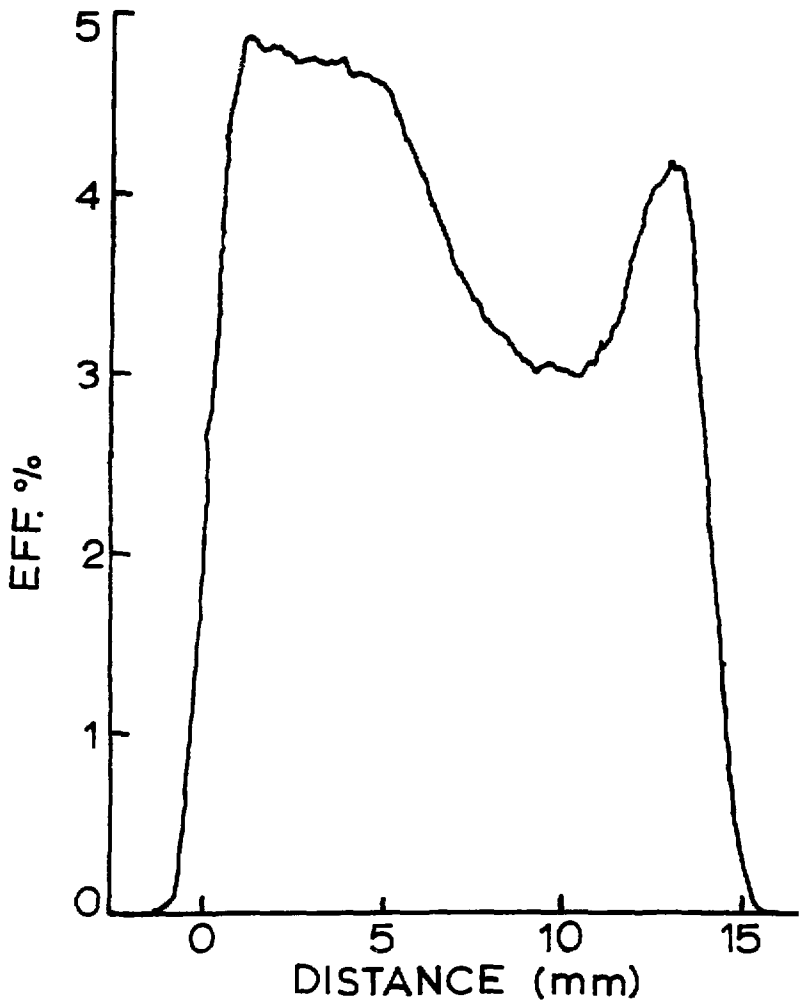

Fig. 3

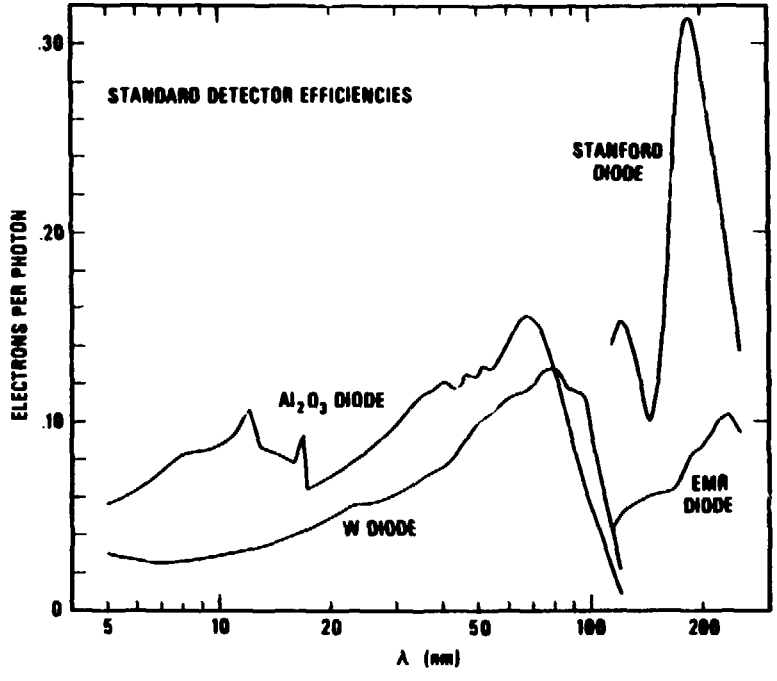
STANDARD DETECTOR EFFICIENCIES
ELECTRONS PER PHOTON
.30
.20
.10
0
5
10
20
50
100
200
λ (nm)
STANFORD DIODE
Al_2O_3 DIODE
W DIODE
EMR DIODE

Fig. 4

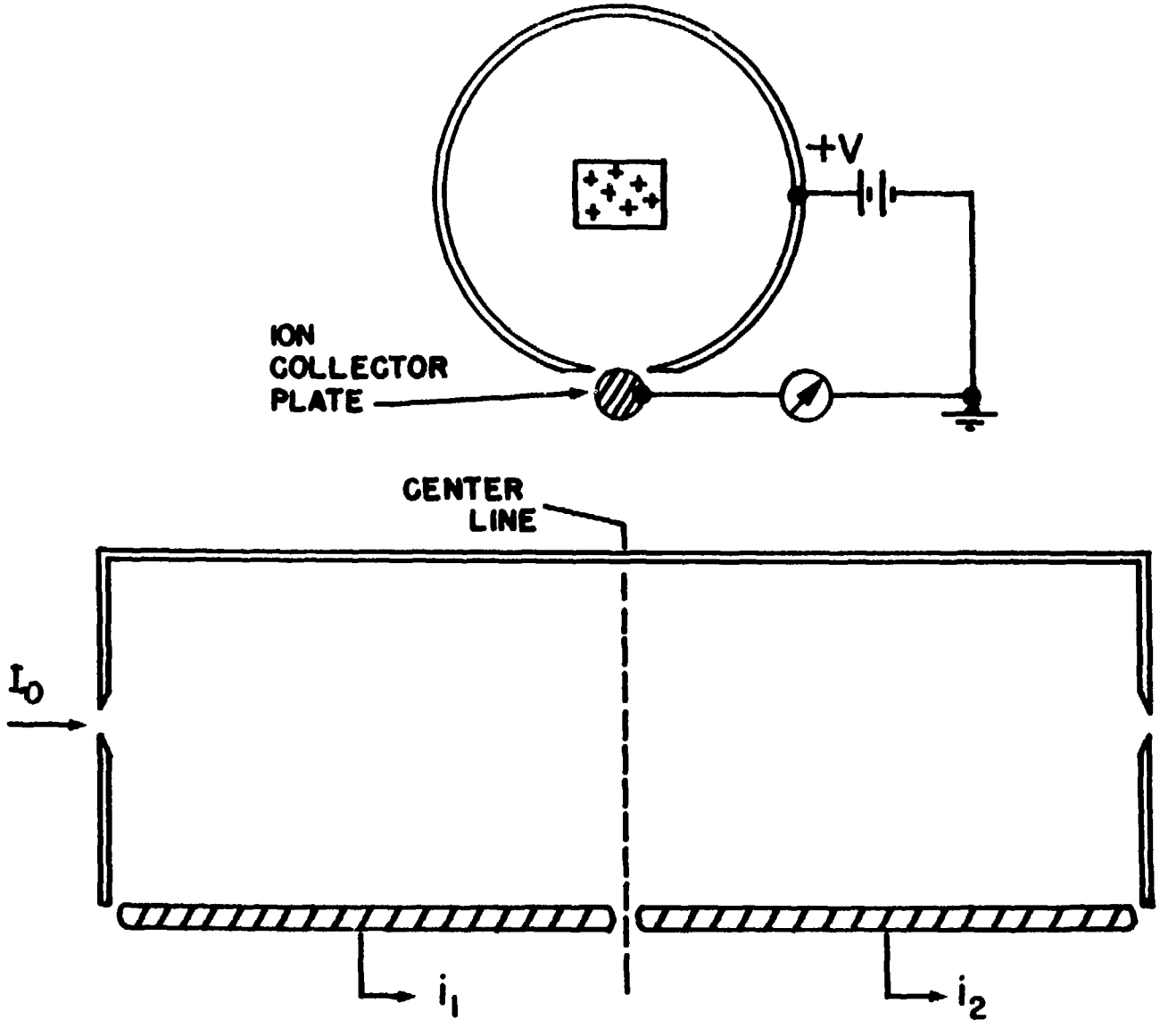

Fig. 5

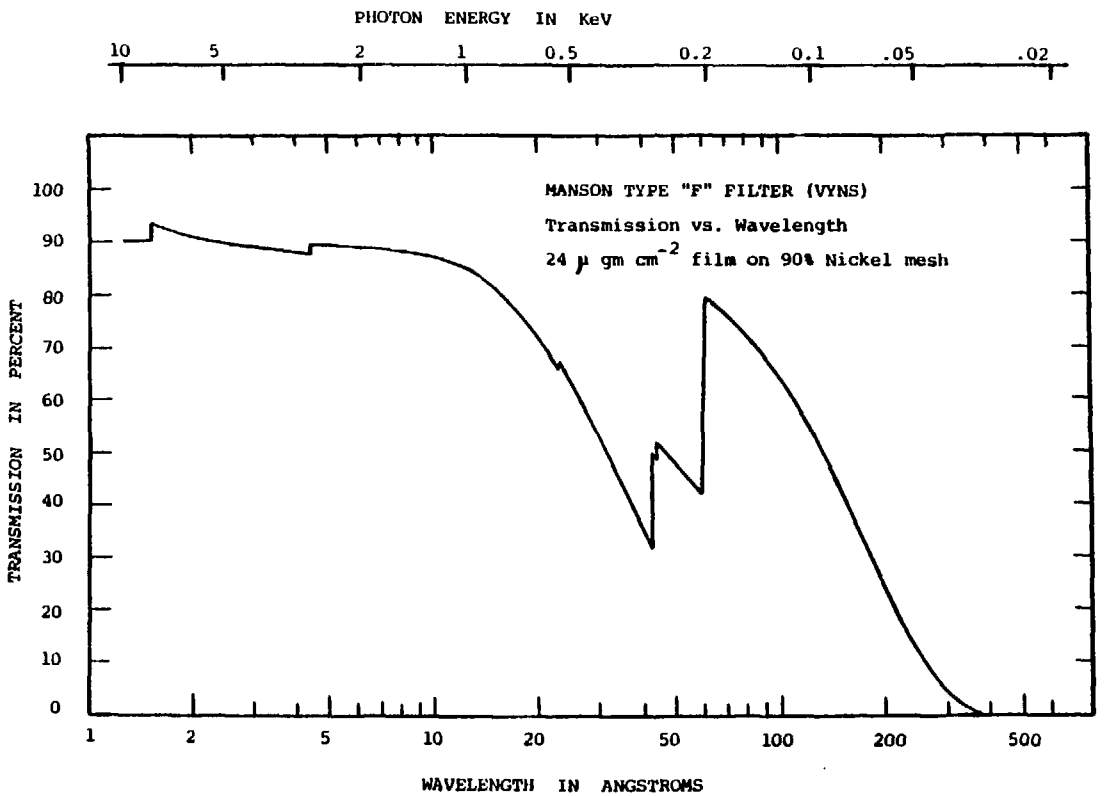
PHOTON ENERGY IN KeV
10
5
2
1
0.5
0.2
0.1
.05
.02
MANSON TYPE "F" FILTER (VYNS)
Transmission vs. Wavelength
24 μ gm cm^{-2} film on 90% Nickel mesh
TRANSMISSION IN PERCENT
100
90
80
70
60
50
40
30
20
10
0
1
2
5
10
20
50
100
200
500
WAVELENGTH IN ANGSTROMS

Fig. 6

ELECTRON SPECTROMETERS

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INTRODUCTION

Measurements made using electron spectrometers can lead to the determination of all the parameters that fully characterise the photoionisation process. The measurements fall into three categories:

a) the angular independent flux of the photoelectrons which leads to the partial cross section,

b) the angular distribution of the photoelectrons, and

c) the spin of the photoelectrons.

The majority of this paper will be concerned with electron energy analysers which can be used to measure both the partial cross section and the angular distribution. The only spectrometer used so far in the measurement of photoelectron spin[1] is the Mott analyser.[2, 3, 4] Briefly, this works on the principle that high energy electrons (100-120 keV) scattered from a thin metal foil, usually gold, exhibit an asymmetry which is related to their spin. The efficiency reported by Heinzmann[3] of 1.5×10^{-3} is as yet too low to allow energy and angle resolved spin measurements with the circularly polarised component of synchrotron radiation as a photon source.

ELECTRON DETECTORS

By far the most commonly used electron detector is the continuous channel electron multiplier (channeltron). Its advantages are its low

noise (typically much less than 1 s^{-1}) and its compactness. The small collection area can be a disadvantage, and the surface is very sensitive to contamination. More recently arrays of channeltrons have been used as in the chevron detector where two arrays are used in series in order to give sufficient gain. This can be used either simply to increase the detection area or as a multiple detector to give spatial information. The latter mode of operation is of great advantage for analysers which have a simple focal plane, or for giving angular distribution information. Descriptions of multiple detector systems and their applicability to various different analysers are given by Carlson[5] and Berkowitz.[6]

ELECTRON ENERGY ANALYSERS

Detailed reviews of electron energy analysers have been given by Sevier,[7] Steklemacher,[8] Wannberg et al.,[9] and Roy and Carette.[10] There are two main types: retarding potential field and dispersive analysers. Retarding potential field analysers have been extensively reviewed by Simpson.[11] They suffer from two major problems, an integral signal and a significant background of secondary electrons, and they are now little used in gas phase work. The signal can be made differential by using a post monochromator.[12, 13] A variant of this idea can be found in the system described by Eastman et al.[14] which consists of an elliptical field low pass filter and a spherical grid high pass filter. This system also makes use of multiple detection, something the retarding potential analysers are well suited to.

The dispersive analysers in commonest use for gas phase work are the hemispherical analyser and the cylindrical mirror analyser. The focusing properties of the hemispherical analyser have been discussed by Purcell,[15]

and there are many examples of it in practical use.[16, 17] It has two-dimensional focusing and a well defined angular acceptance which makes it very useful for angular distribution measurements. Since the entrance and exit slits are not in equipotential planes, some thought must be given to the effects of the fringing fields. Methods of correction for this and other analysers are discussed by Herzog,[18] and Wollnick and Ewald.[19] It is also common practice to use electron lenses[20] to match the object and image to the entrance and exit slits, and to provide a means of changing the electron energy prior to analysis, so that the analyser can be operated at a constant pass energy and hence at constant bandpass.

The cylindrical mirror analyser[21] used for gas phase work has first order slit-to-slit focusing and accepts a cone of electrons making an angle of 54^0 44' with the axis. Aligning the analyser axis along either of the two axes of the synchrotron radiation ellipse, or along the photon beam direction, allows the partial cross sections to be measured without requiring knowledge of the angular distribution of the electrons or the polarisation of the radiation.[22] If the full 360^0 angular acceptance is not utilized, care must be taken to ensure that the symmetry of the segments used is such that the independence of the angular distribution and the polarisation is maintained. The large angular acceptance gives an advantage over the hemispherical analyser, but means that the interaction region is buried inside the inner cylinder. This can be overcome by using only a sector of the full analyser[23] which still retains a considerable solid angle advantage. Pre-retardation/acceleration of the electrons is feasible with the cylindrical mirror analyser, but good matching between the source and the slit is difficult.

The parallel plate analyser has in general not been used for gas phase work either in its first order[24] or second order[25] focusing designs. Its advantages are its ease of construction and its simple focal plane which introduces the possibility of multiple detection. The 127^0 cylindrical analyser[26] has been used for angular distribution studies.[27] Though it has only one dimensional focusing, it is well matched to the line source provided by synchrotron radiation. The pill box,[28] or Bessel box, has also recently been used for angular distribution measurements.[29] Mechanically, this is one of the simplest analysers and this, combined with its compactness, make it a useful alternative to the more conventional instruments.

The capability of scanning the entire energy spectrum at once makes the time of flight analyser attactive. Rosenberg et al.[30] have used such an analyser at SSRL. The resolution is limited by both the time structure of the synchrotron beam and the speed of the detection system. The need for good time structure in the photon beam invariably means operating the storage ring in single bunch mode.

All the dispersive analysers are insensitive to very low energy electrons. For studies of threshold photoionisation several zero energy analysers have been described.[31, 32] In these the zero energy electrons are accelerated at right angles to the photon beam. The higher energy electrons, which will have greater divergence after acceleration, can be discriminated against by using an array of collimators[32] or by subsequent energy analysis.[32]

With all electron spectrometers the limits to the attainable transmission and resolution are set by surface potentials, secondary emission,

and stray magnetic fields. There does not seem to be a clear consensus as to which material or coating is best to minimize the surface potentials and secondary emission, though Schulz[33] suggests that molybdenum may give the most desirable surface. It is important to keep the surfaces free from contamination, especially from anything that may produce an insulating film. The magnetic field problem can be particularly severe in a storage ring environment. As well as the usual shielding methods, Helmholtz coils[34] and mu-metal,[35] additional shielding may be needed for ion pumps and for the fringing fields from the dipole magnets.

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BNL PLANS FOR ATOMIC PHYSICS AT THE NSLS*

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I would like to describe very briefly here the present plans for atomic physics experiments at the NSLS which are being developed by Brant Johnson, Don Gregory and myself. It must first be emphasized that we have a very definite idea of what role we should play at the NSLS. Our BNL group is much too small to think of itself in terms of carrying out an exclusively in-house research effort. Rather, we see ourselves as playing an essential role as a catalyst, or even part of the NSLS apparatus, in making available experimental equipment and assistance to outside users who want to come to BNL to do atomic physics experiments. This assistance could be given either in terms of an actual collaboration or more generally, help in showing people how to find their way around Brookhaven. This is not entirely altruistic on our part. We will benefit from having the best possible atomic physics experiments at the NSLS in terms of pure intellectual stimulation, in the ability to do larger-scale and more complex experiments with the bigger groups gained by collaboration, and by the availability of a wider range of experimental equipment than we can afford ourselves. So, we hope that we will hear from some of you when, or before, the NSLS comes into operation.

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We have formed a Participating Research Team (PRT) for doing experiments at the x-ray ring. Presently, this group includes Ted Kruse from Rutgers and Val Kostroun from Cornell. Generally, our interest is to put together a crossed beams experiment which will permit us to excite or ionize beams from a variety of sources of heavy ions. These will be difficult experiments, but seem to have reasonable rates even with rather modest assumptions on photon and ion fluxes. Initially, we plan to use rather high current conventional sources. Ultimately we hope to use an electron beam ion source (EBIS) which Kostroun is building at Cornell, perhaps coupling it with a storage ring to increase the average intensity. We could thus study something like photoionization not only as a function of photon energy, but also as a function of charge state. Some further details on the EBIS source and the problems of beam handling are given in the contributions of Kostroun and Kruse elsewhere in this report.

The PRT proposal for this work was sent to the NSLS program committee and approved in January 1980 for inclusion in the second group of dedicated beam lines to be installed at the NSLS. We have requested funds from DOE for such a beam line, but have no way, naturally, of telling whether we will be successful. In any case, since we presently have no money, our inclusion in the second group of beam lines is very sensible. A copy of the PRT proposal is included here, as an appendix to this section.

Please note that we do not plan to sit idly until we have our dedicated atomic line and full complement of equipment. Instead we plan to obtain sufficient time on funded beam lines of the facility or other PRTs to enable us to carry out comparatively straightforward experiments,

such as photoabsorption measurements with a differentially pumped gas target or with beams from an ion source of conventional design.

We plan a rather similar program on the UV ring. Here we will work as members of the PRT on the gas phase beam line described by Robb Grover in his contribution to this report. Our principal interest lies in crossed beam experiments, particularly, studies of the photoionization of negative ions. In this case we will try to benefit from the presence at BNL of several groups who are generous with gifts of their expertise and hardware. There are two groups, the Tandem group of Peter Thieberger and the high current ion source group of Krsto Prelec and Theo Sluyters who have volunteered to help us and who have excellent capabilities in producing and handling high current negative ion beams. We hope that we will be able to assemble enough equipment from around the laboratory to mount an experiment during the early days of operation of the UV ring.

It should be quite clear that we have undertaken a large project. We hope that there will be a few more brave souls whose help can be enlisted as collaborators to share the present work and future thrills of Atomic Physics at the NSLS.

An Atomic Physics Program for the NSLS X-Ray Ring

I. Introduction

Several areas of present day experimental atomic physics have benefited greatly from recent technological advances in ion sources and accelerators. Tandem Van de Graaff accelerators have made feasible a great variety of experiments in fields as diverse as beam-foil spectroscopy (BFS) and Lamb shift experiments by providing relatively intense beams of highly-ionized atoms throughout the periodic table. Research in ion source technology has recently begun to be successful in fabricating ion sources capable of generating highly stripped ions at essentially zero energy so that it is now beginning to be possible to select any element in a given charge state at a given velocity for a particular experiment. We propose here to couple the advances of the past decade in ion source technology with the copious supply of x-ray photons from the NSLS to produce an atomic physics facility which will use the photons as a delicate probe of these ionized atoms and which will make possible a variety of new, interesting, and unique experiments in atomic physics. We discuss briefly below some of the physics that can be done, outline the experimental apparatus that will be needed, and discuss the organization of the PRT and its relationship to the wider community of atomic physicists in the United States.

Such a facility will make possible experiments which complement and extend both the work that is done with the heavy ion beams from the Brookhave tandem facility and that which will be possible with the Windowless Gas Phase Beam Line to be available on the NSLS UV ring. From the scientific standpoint the atomic physics results will advance the state of knowledge used for basic atomic theory and will also have significant implications for work in astrophysics and plasma physics as well as giving insights into the problems of molecular and solid state physics.

II. Physics Program

Our intent is to couple the NSLS with a high current ion source to provide for crossed photon-heavy ion beam experiments to study a very wide variety of ionic species. Experiments of this type are complex and must be carried out with great care. It is almost mandatory that the experimental apparatus be placed in permanent positions to preserve the necessary geometrical precision, thus requiring a dedicated beam position, although the beam line could possibly be shared with other experiments. When this apparatus is operational, it will be possible to make precision measurements on the properties of isolated, single atoms, using a high intensity, polarized, monoergic beam of photons from the NSLS as a precise probe. These experiments cannot now be performed and should represent a great new opportunity for measurements in photoabsorption, photoelectron spectroscopy, photoelectron angular distributions, x-ray spectroscopy, fluorescence yields, reaction mechanisms, etc. The new ion source technology will provide copious quantities of highly ionized atoms. By making an appropriate choice of photon energy to neatly pluck electrons from particular shells, the ions will be selectively excited from their ground states. This contrasts strongly with the usual situation in BFS or other laboratory light sources where a violent excitation process generally excites many electrons. Results from these experiments

will be extremely useful for the understanding of such things as atomic processes in high temperature plasmas, either in stars or in the laboratory, and in serving as a fundamental starting point for the understanding of more complex phenomena in molecular or condensed matter interactions.

This facility will be used not only by members of the present PRT, but in the long run by some larger number of scientists who will originate their own experimental programs. It is our view that the best way to proceed towards this objective is to start with our own experiments and to add and enlarge the range of work with further workers as the apparatus is developed and its capabilities are demonstrated. For this reason we will try to concentrate here on some areas that relate to work currently in progress at the BNL tandem facility and which can be extended and complemented at the NSLS in a significant way.

One type of experiment that we plan to pursue is the study of the properties of levels in elements which are of crucial interest for tokamak construction, such as C, O, Ti, Fe, Cr, and Ni. It will be possible to obtain data on the probabilities for exciting these levels which will be extremely useful in calculating energy losses from the tokamak plasmas. Measurements of lifetimes of metastable states in these ions, which are of great interest for plasma diagnostics both for tokamaks and in astrophysics, will be made possible and convenient for the first time. Lifetimes of states in a few times ionized atoms are also of basic importance in astrophysics for use in the development of stellar models. A particularly attractive thought is to use a storage ring or ion trap at the NSLS for long term (> 1 ns) storage of excited ions so that the decay of metastable states can be determined. These measurements are not now feasible. The most widely applied present method for measuring lifetimes is the use of beam-foil spectroscopy, a method which is plagued with experimental problems arising from the nonselective excitation process. The NSLS can be used to make lifetime measurements in a regime which complements BFS; that is for lifetime in the region longer than 1 ns.

It is our belief that research in these and other areas will provide a substantial foundation for an extensive program in atomic physics at the NSLS. Furthermore, as the experimental apparatus is implemented, we expect that the versatility of the equipment and range of possible experiments will attract many outside university users.

III. Experimental Apparatus

The experimental apparatus to be used consists of: (1) front end connection to NSLS and monochromator; (2) interaction chamber; (3) ion sources to produce the desired beams of heavy ions; and (4) electron and photon spectrometers. The experiments with crossed beams are intrinsically ones with low counting rates where care must be taken to maintain the charge-state purity of the ion beams. Hence, the design and execution of the experimental plan must be done very carefully.

Requirements on the photon collimator are conflicting since high resolution and small energy spread are desired for experiments such as photoelectron spectroscopy, but where the highest possible intensity is needed because of the low rates in a crossed-beam experiment. The most important factor is the intensity, and it will be advisable to design for only medium resolution as a result. The interaction chamber is relatively straightforward with the main requirements being provision of numerous ports to allow for the use of a variety of spectrometers. Vacuums in the 10^{-10} Torr range will be needed to eliminate charge changing collisions prior to the interaction region. The choice of detection equipment will depend on the type of experiment to be done so that a variety of detectors will be needed. A 2.2 m grazing incidence spectrometer for UV work will be available, as will a curved crystal x-ray spectrometer, normal incidence spectrometer, and simple x-ray spectrometer. We expect to have several ion sources available. A Danphysik Model 910 is available and provides ion beams with intensities as high as 100 μA. This source will be very suitable for initial experiments. An electron beam ion source (EBIS) is also being constructed at Cornell and will produce highly ionized beams of light elements, but with much lower intensities. This source will be used after a set of initial tests and start-up experiments.

IV. Participating Research Team Members

The group of participating research team members now involves the following scientists:

V. O. Kostroun - Cornell
T. H. Kruse - Rutgers
D. C. Gregory - Brookhaven
B. M. Johnson - Brookhaven
K. W. Jones - Brookhaven

We expect that work on this project at the NSLS will take a major share (∿ 50%) of the total research effort by each participant. At the present time we plan to carry out the work on the ion beam apparatus at Rutgers (high current sources) and Cornell (EBIS) and then move the equipment to the NSLS when it is operational. The Brookhaven group will concentrate on the problems of the front end, monochromator, interaction chamber and detector.

Funds will also be requested from DOE in FY 1982 for additional scientific and technical personnel for the project. Some initial encouragement for such a request has been received from DOE.

Possible Future Experiments in Atomic Physics Utilizing Synchrotron Radiation

by

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The following survey is limited to processes in which a single photon is absorbed and either photon attenuation is measured or the end products following absorption are detected. Furthermore, only interactions with free atoms (or positive ions) in their ground states are considered.

The absorption process is represented by the diagram given below:

	$h\nu$ +	A (or A^+)	e + A^+ (or A^{+n})
	intensity	density	further emission of photons or electrons
	energy	energy (for beams)	intensity
Key parameters	direction	direction (for beams)	energy
	polarization	polarization	direction
	timing	angular momentum	polarization angular momentum timing

The types of experiments that might be performed in the future are considered in three categories as listed below.

A. Experiments designed to measure cross sections for absorption or partial cross sections for absorption from subshells over a broad spectral range.

B. Experiments which explore interesting effects in particular spectral ranges, particularly near ionization thresholds and in regions where autoionizing resonances occur.

C. Experiments which try to explore a particular aspect of atomic dynamics by specifying some of the parameters of the incident beam, target or detected photons or electrons listed above.

Some possible directions in each of these categories will be considered.

A. Cross Section Measurements and Absorption Spectroscopy

Due to the fact that it is difficult to obtain atoms in the free state, our knowledge of photon attenuation cross sections for free atoms is fragmentary. Table 1, taken from Ref. 1, lists the state of our knowledge as of 1975. Progress since then has consisted mainly in extending the table to a few more elements and to making absolute measurements in given spectral ranges of some of the elements in Table 1.

Figure 1 (from Ref. 2) shows a breakdown of the total absorption cross sections for Neon into its component contributions. Similar data is now available for other rare gases, but not for any other atoms.

The high fluxes available at NSLS should make it possible to extend our knowledge of absorption cross sections both in spectral range and in the number of elements covered via absorption spectroscopy. It should also be possible to extend our knowledge of subshell cross sections to free atoms other than the rare gases via photoelectron spectroscopy. Such experiments have already been done using line sources (3).

To date there have been no direct measurements of the photoionization of positive ions. A possible technique for doing this is to perform a crossed beam experiment and collect multiply charged ions in a mass spectrometer. Such experiments are perfectly feasible with the high fluxes available at NSLS and would result in absolute cross sections. The technique is essentially the same as is used to determine electron impact cross sections for ions (4).

B. High Resolution and Near Threshold Spectroscopy

Work in the 1960's with synchrotron light led to the discovery that in atoms two-electron resonances occur between ionization thresholds. The study of such resonances has led to a better understanding of both the correlation effects in initial states and of the autoionization process. The study of such resonances is a continuing effort. All of the spectra listed in Table 1 show such structure. Most of our knowledge of such effects is in the VUV and soft X-ray region (principally below 100 eV). The key to extending our knowledge of these effects to both higher energies and other atomic species is high resolution absorption spectroscopy.

The availability of intense tunable sources has led to more detailed studies of processes occurring near ionization thresholds. The principal new development is that it is now possible to study with moderately high resolution both the electrons emitted by photoionization (or Auger processes) and the fluorescence produced by inner shell vacancy formation with the exciting photon beam tuned in the vicinity of a particular ionization threshold. Such doubly differential experiments (energy resolution in both the photon beam and for ejected photons or electrons) have only recently been attempted in the near threshold region (5,6,7). The feasibility of experiments of this type opens up a new field (Near Threshold Differential Spectroscopy) which will undoubtedly lead to some exciting new atomic physics. When an inner shell vacancy is just barely created (or not created) the electron correlation is enhanced. Just how this enhanced correlation affects the decay products remains to be discovered.

C. Atomic Dynamics Experiments

In terms of the key parameters listed above, the type of experiments described in A and B consider only energy (either of the incident beam or of the end products) as a key variable. Basically, one is limited in energy resolution by intensity and target density. A wide range of specialized experiments can be considered which attempt to exploit the other parameters, some of which will be considered below.

1. Directional Photoelectron Spectroscopy

Energy resolution in both incident beam and electron detection plus measurement of the relative direction of photon polarization and electron direction.

2. Polarized Photoelectron Spectroscopy

Incident beam polarized, detection of polarization of photoelectrons.

3. Alignment Spectroscopy

Detection of fluorescence and its polarization following inner shell ionization.

4. Stark Spectroscopy near Ionization Thresholds

Experiments of the above types have already been performed. Directional electron spectroscopy is rather an old technique, but only recently has it been possible to obtain reasonably good energy resolution in all three variables (incident and final energy and electron direction). The other experiments are described in Refs. 8-10.

Other types of experiments which should be considered are:

5. Time Resolved Measurements

The bunching of photons in a storage ring provides a time signal which can be exploited to provide information on the time dependence of atomic processes. Although inner shell processes generally are too fast to follow

in detail, it is worthwhile considering time resolved experiments. One possibility would be to measure the relatively long times required for the formation of multiply charged ions (either via fluorescence or ion collection) which form the end product of a vacancy cascade when an inner shell vacancy is produced.

6. Crossed and Merged Beam Experiments

Experiments with neutral (or ion) beams could, if sufficient column density were obtained, open up a Pandora's box of possible interesting experiments since the beam axis provides another axis of orientation. For experiments using the storage ring light merging beams provide a useful way to improve the effective interaction volume since the important direction for photon interactions is the polarization direction.

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TABLE 1: ATOMS FOR WHICH ABSORPTION SPECTRA AND/OR CROSS SECTIONS ARE AVAILABLE. THE NUMBERS IN PARENTHESES REPRESENT THE WAVELENGTH RANGE IN ANGSTROMS AND THE ASTERIX INDICATES ONLY PHOTOGRAPHIC ABSORPTION SPECTRA AVAILABLE

Closed Shells

s^2, s^2p^6

He (44-524)
Ne (1.5-600)
Ar (1.5-800)
Kr (1.5-890)
Xe (1.5-1030)

s^2s^2, p^6s^2

* Be (500-2000)
Mg (500-2000)
Ca (10-120), (350-2028)
* Sr (40-95), (1640-2200)
Ba (10-150), (350-1000), (1700-2450)

$d^{10}s^2$

Zn (247-1320)
Cd (400-1450)
Hg (20-120), (172-1188)

ds^2, $f^nd^os^2$

* La (320-1000)
* Ce (10-120)
* Pr (320-1000)
* Nd (320-1000)
* Sm (320-1000)
* Eu (320-1000)
* Dy (320-1000)
* Ho (320-1000)
* Er (320-1000)
* Tm (320-1000)
* Yb (320-1000)

ds^2

* U (320-1000)

d^5s^2

* Mn (100-300)

Open Shells

s^2p

Al (1758-2100)
Ga (1480-2100)
In (350-1000), (1600-2200)
Tl (10-120), (1400-2100)

s^2p^2

Si (1250-1550)
Pb (10-120), (350-2500)

s^2p^3

N (400-900)

s^2p^4

O (400-1000)
S (900-1830)

s^2p^5

* F (600-1500)
* Cl (320-1000)
* Br (600-1500)
* I (600-1500)

s^2s, p^6s

Li (170-210), (500-2500)
Na (150-2500)
K (10-120), (600-2860)
Rb (10-120), (1000-3500)
Cs (10-3500)

$d^{10}s$

* Cu (350-1400)
* Ag (350-1400)

d^5s

* Cr (100-300)

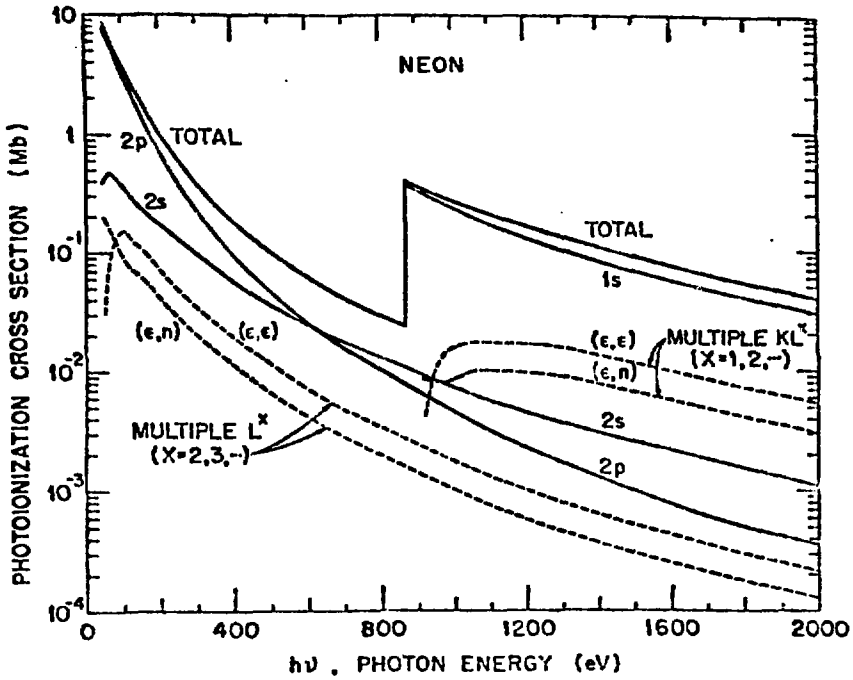

Fig. 1. Partition of total photoionization cross section of neon into its components of single ionization in 2p, 2s, and 1s subshells, multiple ionization, and simultaneous excitation and ionization in the various subshells (ref. 2).

"Applications of Atomic and Molecular Synchrotron Experiments to Condensed Matter Physics"

J. W. Davenport

Synchrotron radiation is expected to be a valuable probe of the geometrical and electronic structure of condensed matter. It appears that the most common experiments will be diffraction and scattering of x-rays and UV photoelectron spectroscopy. To interpret these experiments it is often useful to separate strictly atomic from solid state effects. Hence atomic and molecular experiments serve to map out the range of phenomena to be expected in the absence of bonding. In addition, an atomic effect such as a resonance which is well understood can be used as a diagnostic tool in studies of the condensed state. Several examples of topics of recent interest are given below. For an overview of synchrotron experiments see ref. 1.

One of the most straightforward experiments to do is EXAFS. Here one measures the x-ray absorption coefficient above a core threshold. Normally it oscillates as a function of photon energy because photoemitted electrons are back scattered from neighboring atoms. The oscillations can be used to obtain the positions of the neighbors. Recently very similar oscillations have been found in calculations on isolated atoms (ref. 2). This could have important implications for EXAFS and should be investigated more fully.

Recently there have been a number of experiments on the photoelectron spectra of nickel and copper (see ref. 3 and references therein). The emission from the 3d electrons is greatly enhanced near the 3p threshold (around 70 eV) and strong shake up satellites are observed both above and

below the threshold. It is not clear at the moment if these effects are atomic in origin, and theories have been offered which do and do not require bonding. It would be useful to have vapor data with which to compare.

Finally, there is the shape resonance which occurs in photoemission from CO about 1 Rydberg above threshold (see ref. 4 and references therein). This resonance is a nearly pure $f\sigma$ state consequently there are definite selection rules for excitation depending on the molecular orientation. The resonance was observed in the gas phase and used to determine the orientation of CO molecules adsorbed on various metal surfaces.

No doubt other examples could be mentioned. These are simply a selection of cases of recent interest.

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Use of Synchrotron Radiation for Development of UV and X-ray Detectors for Particle and Nuclear Physics

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A synchrotron radiation light source can provide a very valuable facility for research in the development of new instrumentation in nuclear and particle physics. The availability of an intense, well-defined beam of UV and x-ray photons of variable frequency will greatly improve the versatility and sophistication of tests in the use of photons in such instrumentation. One example is the extensive use of Cerenkov radiation in particle physics experiments. A synchrotron radiation beam will greatly facilitate the study of UV reflectors and refractors for the refinement of such devices. Other forms of photon emission such as transition radiation, bremmsstrahlung and indeed synchrotron radiation itself can be (or have been) effectively used in the detection and recognition of particles; and the use of a synchrotron radiation beam can greatly enhance developments in such instrumentation. In the area of x-ray radiation, a variable frequency x-ray source will be very handy in the development of monochrometers or spectrometers, for example those using diffraction from bent or flat crystals for high precision and high resolution studies of exotic atoms[1,2,3,4] and nuclear γ-rays in the lower energy region. In current experiments involving very low Z exotic atoms such as in the search for the 2S state of muonic hydrogen,[5,6] development of better detectors in the 2keV region is highly desirable and the use of synchrotron radiation can certainly facilitate such efforts.

While one can not foresee all the developments made possible by the use of such a powerful new tool as a synchrotron radiation source, it is certainly evident that the importance of such possibilities should not be overlooked. In the history of each area of physics, a flurry of advances often follows each significant development in instrumentation.

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POLARIZATION OF PHOTOELECTRONS PRODUCED FROM ATOMS BY SYNCHROTRON RADIATION

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The polarization of photoelectrons from atoms has proved to be an important tool for studying correlation effects in atoms, as well as relativistic effects such as the spin-orbit interaction. Extensive experimental[1-4] and theoretical[5,6] studies have been made of the Fano effect,[7] which is the production of polarized electrons by photoionization of unpolarized atoms by circularly polarized light. The experiments have dealt mostly with alkali atoms and with photon energies slightly above the ionization thresholds.

Recently, considerable advances have been made in the study of photoionization processes. The experimental work of Heinzmann et al.[8-11] agree very well with the theoretical treatment of Huang et al.[12-15] using the relativistic random-phase approximation.[16] Particularly, a pioneering experiment[9] has been done on xenon using synchrotron radiation in the vuv region with photon energies up to about 50 eV. The measured polarization of the photoelectrons is in good agreement with the calculated values.

The study of photoionization processes has potential applications in the development of polarized electron sources[17,18] with high intensity or high polarization for high energy particle physics research.[19,20] For example, it might be possible to produce an intense polarized electron beam with typical polarization of 60-80% arising from autoionization states at particular autoionization resonance frequencies. It may also be possible to make such an electron source by photoionizing outer $p_{1/2}$ or $s_{1/2}$ subshells of rare gases.[21,22] The use of synchrotron radiation can greatly enhance such studies.

Consequently, it would be of great interest to pursue this new field of experimentation and to compare the results with the theoretical predictions. It can be anticipated, as is often true in physics, that polarization measurements will provide crucial data to supplement data on total and differential cross sections. The types of measurements that could be made include the following variations:

(1) Photons-linearly, elliptically, or circularly polarized with energies from uv to x-rays (10 eV to 10 keV).

(2) Polarized or unpolarized atomic targets, both low Z and high Z.

(3) Polarization of photoelectrons, transverse or longitudinal, as a function of production angle.

(4) Polarization of residual ions.

Specifically, photoionization of polarized atomic beams, which can readily be produced,[23] has never been measured. As another example, the photoelectron polarization for the xenon atom could be measured for all shells.

The technique of the experiment would be similar to the experiment at Bonn.[9] An atomic beam would be used, which might also be polarized. The polarization of the photoelectrons would be measured by Mott scattering with the Mott scatterer at ~100 kV potential and the photoelectron source and the detection of the Mott scattered electrons at near ground potential.[24] The powerful and versatile source of synchrotron radiation to be provided by the BNL NSLS should be ideal for these important experiments.

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NEGATIVE IONS, PRODUCTION OF SLOW HIGH-q IONS, COLLISIONS WITH INNER-SHELL EXCITED TARGETS USING SYNCHROTRON RADIATION.

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Tunable XUV radiation is important in atomic and molecular physics for the basic reason that the scale size for electronic binding energies in atoms and molecules is the Rydberg energy unit $hcR = \frac{1}{2}e^2/a_o$ 13.6 eV, corresponding to the hydrogen atom photoelectric threshold wavelength near 910Å. All atoms and molecules will show outer or inner-shell electronic photoabsorption near or somewhat below this wavelength. The combination of high intensity (compared with conventional continuum sources) with monochromaticity and wide-range tunability is needed for systematic absorption spectroscopy of atomic core-excited states. The pioneering work on precision spectroscopy of autoionizing series in atoms was done a number of years ago[1] but there is still considerable interest in this kind of work which should be greatly facilitated with synchrotron radiation. The work is needed for a better understanding of electron-correlation effects in many-electron atoms and of the nature of many-body discrete states embedded in a single-particle continuum. Even in a two-electron system, double electron excitation cannot occur with electric-dipole photons without electron correlation. Strong effects have been observed in both helium and H^- photoionization[2].

In addition to the "obvious" uses of synchrotron radiation for XUV

absorption spectroscopy of atomic and molecular targets, it seems to me there are at least three promising research areas in atomic physics that have received very little attention as yet. These are: (1) XUV excitation of "two-body" negative-ion autoionizing states; (2) production of low-velocity ions of high charge states by inner-shell ionization with synchrotron radiation followed by Auger cascade; and (3) atomic collision experiments at low velocity using selectively inner-shell-photoionized target atoms.

Negative ions: multiple thresholds with multiplet structure have been observed in the visible photodetachment spectrum of a number of negative ions, primarily by laser photodetachment[3]. A rich structure has been observed in the photodetachment spectrum of the simplest negative ion in the XUV region as well, by "colliding" a UV laser beam with an 800MeV H^- beam and making use of the relativistic Doppler shift to produce barycentric photons in the 900Å range.[3a] The method is not general because of the unavailability of relativistic beams of heavier negative ions. This kind of work could be extended to other ions by using synchrotron radiation and low velocity negative ion beams. Two-electron resonances embedded in the one-electron continuum should be abundant and of particular interest when excited from a negative-ion ground state.

High charge states at low velocity: Synchrotron radiation offers the possibility of producing heavy ions in high charge states at low temperatures,[4] which could be important for example in accelerators

designed to produce beams of highly-stripped ions with low emittance. The use of monochromatic x rays of XUV radiation with photon energy just above an absorption edge will produce an inner-shell vacancy, followed by an Auger cascade. In low to medium-Z elements, the dominant mechanism for filling the vacancy will be Auger-electron emission rather than x-ray emission. This will usually lead to two vacancies in the next higher shell and the cascade can continue until the outer shell of the atom is reached. In a medium-Z element with full K, L, M and N-shells, for example, each initial K-vacancy will usually lead to the ejection of a total of seven electrons, resulting in a final ion charge state of +8. Electron "shake-off" processes[5] will further substantially increase the final charge state. Using x rays to produce an initial L vacancy in Hg (Z=80), for example, would be expected to yield ions up to charge +17 with a mean charge of +9.8 (see Ref. 5). The resulting slow ions would be useful in spectroscopic studies and perhaps in the production of high-quality accelerated beams for ion-beam fusion.

Collisions with ions having selected inner-shell vacancies: almost no work of this kind has been done. There was one study of "carambole" collisions in gases (Ar^+ on Cl_2)[6] involving excitation of an L-shell vacancy in Ar by the first Cl atom, followed by a vacancy transfer to the second Cl and there has been some exploratory work involving multiple collisions in solids[7]. Synchrotron radiation in the 50-100Å range would make possible the production of slow target ions of low Z (e.g. Ar) with specific L-shell vacancies (e.g. $2p_{1/2}$ or $2p_{3/2}$).* Quasimolecular models of slow heavy-particle collisions (ion-atom)

*The short lifetimes of such states would make these experiments difficult but not necessarily impossible, for example, if solid targets were used. Vacancy-sharing studies in molecular targets might also be possible.

could be tested using these target ions in a detail not possible before. Absorption experiments involving molecular-orbital transitions within a collisional quasimolecule may also be feasible with intense XUV sources. Such experiments have previously been done only in emission.[8]

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GENERAL DISCUSSION SESSION

Chairman: B. Crasemann (University of Oregon)

Several discussion sessions were held, in addition to the extensive commentary made during and after formal presentations. In general, we did not try to reproduce this in the workshop proceedings. However, in one session the participants were asked to describe what they considered to be an important question to be addressed at the NSLS. This turned out to be a particularly stimulating session, and we thought it worthwhile to include a transcript of these remarks. We note, as a caveat to the reader, that the transcript was edited to improve readability and that the speakers have not been asked to approve this version. All the good ideas are to be attributed to the speakers, while the errors are entirely the responsibility of the Editors.

B. CRASEMANN (University of Oregon): We had a little strategy meeting for a few minutes just now and thought it would be most helpful if we first concentrated on very broad experimental areas that deserve investigation and where it is likely that the synchrotron radiation facility will be helpful. Then we can pinpoint individual experiments, instrumentation, and specific plans. But, first it's a question of just being as broad and general as possible and identifying areas of problems. I think it is generally recognized that the frontiers in atomic physics are really in the area of many-body aspects, relativity, and QED. Just to go backwards--for QED the Lamb shift measurements that are done on other types of machines are relevant. Even atomic problems like measuring level energies very accurately, which seem a little dull, are actually quite

relevant. That is because such problems as the effect of screening on self-energies are something that even Wally Johnson doesn't dare tackle beyond the innermost shells. There are certainly interesting and unknown things to be found. Relativistic effects--well, again it's a question of how much of the right operator you throw in. It is quite clear that studies of these forbidden transitions in lithium-like atoms are the best known examples. But these are funny states that can't go except by relativity. These are extremely interesting systems that are accessible here. Many-body is of course the main thing. Everybody knows that Hartree-Fock theory is limited and that only Hugh Kelly knows how to go about making the diagrams. Let's try something we learned from Walter Meyerhof who did this at a workshop we had in New London a few weeks ago and some of you were there. It seemed to work well. Maybe we should go around the room and just ask each person who is left here to suggest his or her ideas as to what really interesting areas might be accessible to investigation by synchrotron radiation experiments.

J. COOPER (National Bureau of Standards): The field that I would like to see exploited very, very much is the thing that you were talking about a couple of days ago: this business of near-threshold spectroscopy. I think this is a field where if you're just forming an inner-shell vacancy or barely forming it, since we really don't know what is happening, that there is really some theory that has to be developed. It is not a question of checking theory. It is a question of how the correlation, when you work very, very near an inner-shell edge, is enhanced by the other electron being in an excited state. There is the possibility that

if you have fluorescent radiation, it is almost the same as that you're exciting near there, so there is a problem of correlation with the radiation that's being scattered and the radiation that you see in the fluorescence. In fact, this is what I think the resonant Raman effect is all about. Normally we think of the excitation mechanism and then study the atom after the excitation has taken place. Here we have to consider the light channel plus the electron in the many-body system of the atom. Usually we study the initial and final states of the many-body atomic system and consider the light coming in as the excitation mechanism. We have to go theoretically a little bit beyond this. Honestly, I don't know how to do it. Perhaps some of the others here have something to say. So this is a very exciting concept, and we can study it by several methods. We can do it by Auger photoelectron spectroscopy, and we can also do it by fluorescence. Another thing that's exciting that hasn't been alluded to is that if you're looking at a low energy Auger process and also have a photo line at some energy above threshold you can tune your photon beam so that your photo line lies exactly on one of your Auger lines. It is then possible to study the correlation between the photoelectron excited out of an inner shell and you have a photoelectron going at some energy; you really reach a place where the electron for some particular multiplet (if you tune your photon energy) has exactly the same energy. Now obviously, there is going to be a correlation there. How you treat it theoretically, I don't know. In the simple picture, it's a two-electron process where two electrons come out at one energy.

B. CRASEMANN: Do you know the Smith experiments?

J. COOPER: Yes, where they went across. But they never studied this in detail. Maybe one can do coincidences on these things. It's very similar to a near-threshold process in electron scattering.

T. CARLSON (Oak Ridge National Laboratory): Actually, John covered my second point already in the terms of the core shells. In fact, I think one of the biggest things that the VUV synchrotron source offers for the first time is a high intensity source in that range for the penultimate shells. So, we really can start doing near-threshold core shells. I think that is a tremendously big frontier. I would like to add a word about molecules because experimentally, very many of the same things are identical to the atomic case so that you can do the same experiments. But, more important, I think that for molecules we have just begun to scratch the surface of understanding how to handle the continuum wave function with a many-centered calculation. I think that the best way to test this understanding is through photoionization photoelectron spectroscopy. Just a little bit of work has been available, and it has been very exciting. Some people may have the idea that we have done a lot of work already on many of the systems, but, as a matter of fact, practically nothing has been done outside perhaps, let's say, the rare-gas atoms. There is just a tremendous amount of work needed, both for other atoms, open-shell atoms, and for molecules over the whole energy range.

R. CHATURVEDI (SUNY, Cortland): The experiment that I have in mind is resonant Raman scattering. In the first talk Dr. Crasemann mentioned that there could be lines longer and narrower than the Lorentz lines. If you can do that with synchrotron radiation, then my feeling is we can

have the tuneable Mössbauer source. If that is possible, even up to 20 or 30 keV, I can see a possibility of using this Mössbauer source and doing some nuclear physics, to study g-factors, for example, of very low-lying nuclear levels.

Y.-K. KIM (Argonne National Laboratory): In the atomic relativistic effect the most important part is the spin-spin interaction of the electrons. For a closed shell, when the total spin becomes zero, that part goes to zero basically, and it doesn't play an important role. So, if you create holes in inner shells, particularly double holes, like two holes in the 1s or two holes in the 2p levels, then the energy levels have to match the theoretical calculations which now have a very large contribution from the non-zero total spin of the open shells. There has been some experiment done in the past with the x-ray light source, but as you know, the probability of creating two 1s holes is very small. So, I say that is one example where you probably can use the very hard x rays to do some experiment and provide some data that will have strong bearing on the relativistic method we use to calculate energy levels.

P. WOODRUFF (University of Wisconsin Synchrotron): Experimentalists have done the rare gasses long enough. There's a vast amount of information on them now. I think the next stage has to be to go to the open-shell atoms, to start getting some information out there where, as Dr. Kim has said, we don't have zero spin any more. In connection with that, to also start measurements on the spin of the photoelectrons. This will require some technical developments in terms of spin analyzers, so that we can not only get the spin of the total photoelectrons ejected, but

also the angular distribution. So you will be able to measure three spin parameters, the partial cross sections, and the angular distribution and really tie down photoionization processes.

K. W. JONES (BNL): I would like to say that we are most interested in doing a crossed beam experiment with a beam from an EBIS-type ion source such as Val Kostroun is building at Cornell and which we hope will be brought down to BNL for use when it is finished. I would like to think that someday we will be able to excite any ion beam in any charge state with photons from the NSLS. As an example of what might be done, I would like to try to measure lifetimes of metastable states of highly ionized iron. This is of interest for plasma diagnostics in tokamaks and is a technical problem that you can't manage at all by use of the conventional technique of beam foil spectroscopy with tandem accelerators.

B. M. JOHNSON (BNL): I also would very much like to see experiments with crossed or merged ion and photon beams. To my knowledge there is only one similar effort along those lines in the world. Ken Dolder is working on similar experiments, but I have been told that he's very busy in other fields, and perhaps is not making as much progress as he would like to in that area. So this could be a unique facility in the world for studying a wide range of experiments that are inaccessible by other means.

J. D. LARSON: I can't speak to the physics, but I would like to comment on the logistics of setting up an experimental apparatus. In my opinion, it would be very wise to acquire sound front-end devices for

your experimental apparatus. There was some concern about costs and my opinion is to spend the money in developing good monochromator vacuum systems and other devices that you're going to need. The experimental apparatus can be crude to begin with, and certainly become refined after the fact, but it's oftentimes difficult to start over again from the synchrotron and rebuild from that point out, so I would suggest the initial hardware be expensive hardware, if that is necessary, and that the cost not be cut in a false economy at that point.

W. SAVIN (New Jersey Institute of Technology): This is all very new physics to me. I really have had no contact before this meeting with any of it. The thing that had interested me most was the crossed-beam experiment. I would like to be able to think about and possibly even work with experiments which would take beams from ion sources in different charge states and have them interact with the synchrotron radiation. I thought that Ken Purser's comments yesterday were really interesting. His techniques to identify the states and conditions for low-counting rate experiments, so you could pick the weak signal out of noise are things which should be thought about. Again, it sounded to me as though there was a great deal of money involved in the equipment and beam lines for something like this.

T. H. KRUSE (Rutgers): I think the crossed ion-photon beam experiments seem particularly interesting since they open up a vast region which has been inaccessible. Along with that idea goes the fact that I think they are on the edge of feasibility even with the high flux synchrotrons and therefore need to be thought about very carefully. It seems to me

there are possibilities, not only with atomic ions, but also with molecular ions which implies that there are possibilities on both rings. One thing which I would like to know more about from people who know more than I do is to what extent should some of these experiments with ion beams be done with electrons instead of photons. Are there specific experiments for which the photons are most appropriate and others which should be left to electron interactions?

D. C. GREGORY (BNL): Continuing Ted's thought about electron and photon relations, perhaps we should think about what experiments could be done either way, not only which experiment could be done best with photons or best with electrons. Are there experiments where the two areas overlap, and can you get similar or even more interesting related information from doing experiments first with photons, and then with electrons?

J. COOPER: I think a strong recommendation that we can give to the crossed-beam people is to try and interact with some of the people that are doing the crossed electron-ion beam experiments and are trying to generate absolute cross sections. There is a fair amount of interest in this now, as a result of the fusion program, and I think there could be interaction between the two efforts that would be very valuable to the people working on the photon-ion beam experiments.

V. KOSTROUN (Cornell): I don't think I can add more to some of the ideas that have been presented about threshold effects, open-shell atoms, excitations of ions. I think the area is open for the types of experiments that can be done. We're beginning to look at ions, photoionization, mass

and charge spectroscopy, that is, to do the expeirments that Tom Carlson started on many years ago. I think that experiments of that nature could be done at the synchrotron and would reveal quite a bit of information about multiple processes at threshold.

D. CHURCH (Texas A & M University): What impressed me I think was the theoretical interest in ions. Although Val and I are both interested in highly charged ions, the interest in singly charged ions, either positive ions or negative ions, seemed to be comparably as great. It seems that if you're going to make a source of ions that those would be the easiest ones to produce and, if the results are useful and interesting, that might be the first experiment to look at. I think the advantage of an ion beam target as opposed to an ion-trapping target is that you have a bigger range of possible experiments. You can do angular distributions and a number of things with an ion beam which you probably would find difficult to do with an ion trap because of the fields which are present. The other thing was, that despite all of the claims that the intensity is high, the intensity when you look at ion beams is low because of low density and relative intensity of the photons. I think it would be useful if one does ion beam experiments to know what the minimum desired resolution is and then try to design some instrumentation which will get the maximum intensity with that resolution.

L. ARMSTRONG (Johns Hopkins): I think a number of very interesting topics have been mentioned that are interesting from a theoretical standpoint. Among them are things such as double photonionization, threshold

effects, and so on. I think a word of warning or perhaps of caution should be given to the experimentalists. That is that calculations in almost all of these areas are extremely difficult to do. Once you start doing experiments, you can probably produce a lot more data than the theoreticians can look at. This is a problem we ran into with an astrophysical workshop we had recently. The experimentalists wanted a lot more data than the theoreticians could really produce. So there should not be great expectations that when you produce a lot of data that the theoreticians are going to be able to explain it rapidly. A lot of these calculations take years to do. An area which I think has only been briefly mentioned by Peter Koch has to do with using multiple light sources, if you will. That is the synchrotron and laser (I see an indignant person here. Steve Manson also mentioned it). There is a lot of work which has been done in multiphoton processes using lasers. A lot of it could be applied to studies using a synchrotron source, that is, where one of the lasers is replaced by the synchrotron source. This then allows you to get into very different sorts of experimental situations than are presently being considered by the laser people. I think that is a field which should be looked at in some detail.

S. T. MANSON (Georgia State University): Well, actually we had a very interesting discussion about some of these problems last night between about 12:30 and 2:00 in the morning. Earlier, you know, we talked about some specifics. What I would like to mention is sort of a general problem which many of the individual areas we've talking about impinge on. That is the three-body continuum Coulomb problem about which we know

essentially nothing and which perhaps is the central problem of atomic physics. Some processes are directly involved with it, like the double photoionization of anything, double photodetachment. But there are also other processes that aren't that directly concerned, but do give some information about it. For example, consider photoionization plus excitation. It's not the same, but it's leading up to it. Another example is just the autoionizing states when you have a core with a double excitation. You can have two electrons that are far away. They are still loosely bound; it is a system that in some sense we know how to treat, but, nevertheless, it does sort of mock-up the three-body continuum Coulomb problem. This is being studied in great detail in lots of quarters right now. The point I am trying to make is that while there are lots of very interesting experiments, I think one thing we can hang our hats on here is a very crucial unsolved problem of physics.

J. R. GROVER (BNL): I want to go back to something that was raised and dismissed in rather short order on Monday and that is the possibility of exciting nuclear levels with the x-ray ring. There is an old game in chemistry called perturbed angular correlations. The point I think is that throughout the periodic table there are many levels which are within reach of the x-ray ring, especially with the wiggler. One can excite these levels and two things occur to me. One is that you get internal conversion in these levels. You make vacancies in the atomic shells and these will subsequently make Auger electrons. You ought to be able to measure the angular correlations of these things. The other is the idea of perturbing the angular correlations by doing something to the atom, or

in the case of my interests, the molecule. The things that will cause the perturbation are the magnetic field at the site of the nucleus, assuming one has one or the electric field gradient. An example of the problem that such a technique might solve (in the moleculr case) might be the cases of the mixed valence compounds such as palladium- where one has a palladium of valence-2 on one side and valence-3 on the other side of the molecule. It's an interesting chemical question. What is the real state of these two metallic ions? Whether they oscillate from 2 to 3, back and forth, or whether one has some kind of quantal blend. This kind of problem could be answered by perturbed angular correlation of a state that lives for a few nanoseconds. So, just a plea for, don't forget the nucleus.

J. A. R. SAMSON (University of Nebraska): Well it's hard to follow Steve...he's just stolen all my experimental ideas, so I would like to start with what I think is probably the most important project that we all have. Now that we've a few theoreticians interested in photoionization, it is up to us to try and keep them interested and keep them busy. But Lloyd said that he can't do all these complicated calculations. Well, I am very glad so many of you are interested in the photoionization. I would like to reiterate what Steve has stolen from my notepad over here, and that is to study the excitation and ionization leading to double ionization with both photoelectron spectroscopy and fluorescence techniques. One very interesting project is to look at the photoionization cross sections of open shell atoms or any atoms other than the rare gases and forget about trying to do it in an absolute fashion. What I propose is that we study

the relative photoionization cross sections and perhaps rather rapidly try to map these cross sections and see what they look like. So if we have something like this, we can perhaps quickly check some of the theoretical calculations. That would be true for both molecules and atoms. One of the major advantages of photoelectron spectroscopy is that we can get branching ratios and, if we know the total cross sections, we can break that down into the partial cross section. If we just do photoelectron spectroscopy, we only get a branching ratio. If we have curve like this, we can now put in the curve of partial cross sections, but we do give the true shape of these partial cross sections. Otherwise we can do almost what we have done with the rare gases, that is, we can break it into all the individual processes. Once we have this as essentially an atlas, it can be used to design some of the more exotic experiments. If you have your crossed beams with ions coming in, it can predict perhaps what energy levels or what photon energies you should be looking at to get some good information. Now an experiment no one has discussed and is a very good experiment that we should be looking at is on some of the autoionizing lines. Experimentally we should be probing with photoelectron spectroscopy. Some of the lines are wide enough if we have the resolution and wave length resolution. I noticed on a chart of planned monochromators for the NSLS that some of the monochromators haven't got high enough resolution for an atomic beam line. Perhaps you should think a little bit about getting high enough wavelength resolution so that one can use the high flux that we have at Brookhaven to probe into something that is, say, half an angstrom wide. I think you do have some

instruments with about .2 Å resolution, but perhaps you should get something a bit better than that. This is an example of doing an experiment and perhaps wasting time trying to find out what is happening before you realize that you're sitting on a resonance. It's probably faster to start mapping out some of these things so you know where you're working.

M. WHITE (BNL): I'd just like to echo the sentiment that photoelectron spectroscopy has been sort of stuck in between yttrium anodes and aluminum. To go up to one kilovolt is an area that photoelectron spectroscopy has been waiting for for a very long time. So anything that we can do will be in virgin territory and give new and interesting experiments. I would particularly like to mention something that hasn't been touched upon specifically and that is the filling of the vacancies at threshold. We have heard something about the resonant Raman effect, but an alternative kind of experiment is that we look at the Auger effect, or the fluorescent filling of the vacancy, and its angular distribution, or in the case of photons, its polarization. Here what we will get is the alignment of the ion produced by the photoionization. That is, we'll get the m_j distribution of the ion versus photon energy. This has a strong dependence near threshold. We're not talking about electrons interacting after the ionization process or an exchange of energy. We're looking at the ion itself. The nice feature of the experiment is that we can do the small Z atoms, and we can look at Auger electrons above 1 keV or so. We can then go to the larger atoms and look at the fluorescence. Both of these experiments are easily done, I would think, because the Auger yield will fall off as we go to higher Z. The other thing is that these experiments

are not sensitive to the phase shifts of the continuum, and thereby only the radial matrix elements, are simpler in a sense theoretically. With this kind of a measurement, in addition to the angular distribution, we can sort out the phase shift from the matrix elements versus photon energy.

J. DELVAILLE (Smithsonian Center for Astrophysics): Well, I suppose in some way I should speak to the needs of physics appropriate to astrophysics, atomic physics appropriate to astrophysics. I don't want to leave the impression that the only thing needed is calibration of instrumentation. Really, I would like to reiterate the plea for crossed-beam experiments. The importance there is for tokamaks and for astrophysics because in a tokamak you have your very own star to work with in the laboratory--a nice thing to have. I would hope some of the elements considered there would be iron, sulfur, chlorine and molybdenum.

C. BROWN (Naval Research Laboratory): My point of view is from things we've been doing with multichannel quantum defect theory to interpret Rydberg states. I think we're making very good progress in describing the discrete states, the autoionized region of two-electron systems, and we are sttempting more complicated ones. The data that we can get from conventional spectrometers and laboratory absorption arrangements are energy levels and parameters related to them, but the things we really need to fill out the picture are the oscillator strengths and line shapes from the autoionizing resonances and discrete states. I think that's really where we're going to make progress with the synchrotron type source. I thnk that high resolution, better than a tenth or hundredth

of an angstrom, is going to found to be necessary, especially if you get to more complex nonalkali-type of things where the interactions among channels are complicated. A lot of the details are concentrated in very small wavelength ranges. So I would say high resolution studies will be very fruitful. I also think that the molecular problems are interesting. The O_2 system has been studied and studied and studied. But the theoretical model for this photo-dissociation is just so incomplete we can't understand it. As a molecule comes apart, the rotational and the vibrational electronic energy all become the same size. We just don't have the right picture of that. We need some theoretical help on that very important problem.

P. KOCH (Yale): Well, on a physics note, I mentioned the other day that one of the things that attracted me was the possibility of using the synchrotron photons to put a lot of energy into a system in a way that electrons and particle impact don't. Namely, there are selection rules involved. One can come along and tickle the system with another couple of electron volts worth of laser energy and thus have the possibility of studying at high resolution very energetic systems (including, possibly, even triply-excited states). Let me withdraw for a second, though, and talk about this thing in the overview. As Bernd mentioned the first day, we are an atomic physics community trying to cohere for the use of the synchrotron radiation sources. A coherent view of things would be very helpful rather than an incoherent view. We are going to try to have to win over some of our colleagues in the laser community and in the rest of the atomic physics community because, I think, as we

start to do experiments in synchrotron radiation we will be judged by our output relative to the investment. These experiments are going to be relatively expensive certainly to get them off the ground because of the high cost of front ends, monochromators and the ultrahigh vacuum systems which have to be compatible with the high vacuum in the ring. So we don't want to just be filling up data tables with lots of interesting little facts; we want to be doing physics. It is important for us to agree what that physics is so that we make an impact. I also have a feeling that we are facing some stiff competition by atomic physicists in other countries who are already well along. So coherence and cooperation rather than fragmentation is something that I look forward to finding in the field.

D. LU (Yale): There are two somewhat vaguely related areas in which the Yale group, headed by Dr. Vernon Hughes, is interested. In the area of basis physics we reflect the sentiment alread voiced by Ms. Woodruff, namely that studying the angular distributions and polarization of photoelectrons would be very interesting. This is an area that has seen some very recent good work done, typified by the report by the group of Heinzmann and Kessler in Physical Review Letters about a year ago. Our interest in this is mostly the Fano effect, the role of the spin-orbit interaction in ejecting the photoelectrons into the continuum, and such basic problems. But we are also interested in the immediate application because our group has a wide range of interests. One of the recent things we did at Stanford was to study the scattering of polarized electrons from polarized proton targets and deep inelastic scattering of

electrons. In this realm, for instance, use of a very good polarized electron beam is very important. I think with the use of a continuous tuneable strong source of photons the development of this type of source is a very interesting thing to pursue. Also in relation to this, I think the sentiment voiced by Dr. Delvaille about the uses in astrophysics for the calibration of instruments and development of other instruments is correct. The x-ray ring obviously has a lot of applications regarding instrumentation and testing of instruments and development of very useful instrumentation for other fields. I myself am involved in x-ray monochromators which are used for high precision studies of pionic and muonic x rays at LAMPF and other places. The availability of such a facility for testing our instruments would be a very valuable opportunity to us.

B. CRASEMANN: I think you made a very important point, that atomic physics is not entirely alone, but very closely related with other fields of physics, and we hadn't really yet emphasized that.

W. SMITH (University of Connecticut): When I made up my position paper in advance, I thought about electron correlation and ionization with simultaneous excitation, so I feel very strongly that these are extremely important problems. One thing that was mentioned was the possibility of doing studies with the VUV ring on negative ions. It is said that the H^- ion, although it is bound only because of electron correlation, has no excited states and that's the end of the discussion. But, in fact, it has the very rich autoionization spectrum which is now being mapped out in detail by using a crossed laser beam and the H^- ion beam

LAMPF at 800 MeV. Recently, measurements on the two-electron photodetachment of H^- have been started. That shows very clear evidence by using motional electric fields of another channel (which I think Steve Manson referred to) where you have one electron emitted, plus an excited hydrogen atom. I think that the extension of this kind of study to other negative ions in the VUV range with the copious sources of negative ions now available of various types, in addition to the very exciting possibility of doing crossed-beams with EBIS and ordinary negative ion sources will be fruitful. There are many negative ions that have been produced now, and I think one ought to take at look at them. Another sort of practical thing that appeals to me and hasn't been discussed too much, except by Tom Carlson, is the possibility of using the synchrotron to produce an inner-shell vacancy and then follow that with an Auger cascade so that you produce cold highly stripped ions that could then be used in a variety of experiments in accelerator ion sources. I think that's something that ought to be looked at pretty seriously.

H. KELLY (University of Virginia): Well, most of the things that I would think of have been covered. But, there is still one topic actually that hasn't been covered too much. In atomic physics there has not been too much work done on photoelectron spectroscopy where you map out partial cross sections, particularly very small partial cross sections. A very good example is a cross section such as the 3s in argon and the ms cross section in other atoms. These cross sections are extremely sensitive probes of correlation effects in the atom. This has really not been mapped out to any great extent. A particular example

that people keep talking about is in xenon where the $4p_{1/2}$ subshell disappears essentially completely due to many-electron effects. It would be very interesting to try to map these cross section out in many systems. Another thing that is somewhat related and that we have heard a lot about--John Cooper talked about it--was photoionization near threshold of a number of systems. Now, I hate to harp on this again, what you have there is mainly an interplay between various forms of double ionization and that needs to be studied in great detail. In other words, to what extent is the Auger not really a simple Auger process? It really is, we know, some sort of process where one photon comes in and two electrons go out. To only a limited extent can that be really interpreted as one electron goes out and a little later one goes down and one goes out. There is a tremendous interference that is going to go on as you come into that range between these various contributions to this double photoionization. Now I would suppose then to analyze that, I am not an experimentalist but you need to look, as John Cooper said earlier in the meeting, at the final product states. You are going to have to look at the amount of double ionization you get and probably energy-analyze the ejected electrons to help you untangle this process. And as Steve Manson now says, the angular distributions are going to help you untangle these things. I think that this is extremely interesting. These effects can be calculated at least in low order. I mean this problem of two electrons in the continuum can be at least crudely calculated. It may be that such experiments as we are talking about will give some interplay between theory and experiment.

The crude calculations will be done, then the experiments and this will stimulate better calculations.

On a rather different subject, Tom Carlson talked about continuum states in molecules, but the types of states he alluded to were mostly electronic continuum states. Charlie Brown already has mentioned the photo-dissociation in O_2, but one process we haven't talked about would be the very complicated photo-dissociation of multi-atom systems: the triatomics and so forth. This would be probably, I would think, a field waiting to be hit by synchrotron radiation. Photoionization with excitation has been mentioned a great deal. To be just a little more specific, there are these very interesting results that we saw by Woodruff and Samson in helium. Those are particularly amenable to calculations, and calculations aren't easy, but they can be done, so there will be a lot of interplay here. Now there is another type of photoionization with excitation that is in more complicated systems where the excitation is a very small excitation. It turns out that there were recently some hints in some solid state experiments of some very interesting atomic effects. These were done in copper. They were trying to see whether there would be satellite lines that you should not see in a closed-shell system such as copper. Essentially what they saw there is that when you photoionize one electron in copper (it's copper-plus actually), one 3d electron goes out and one goes up to a 4s level which is extremely close-lying. This cross section, it turns out, also can have great resonance effects, which wouldn't exist at that same energy range in the orginary 3d cross section. So there should perhaps be in systems of

of this type very huge effects of photoionization with excitation. To simply understand the photoabsorption cross section you are going to have to understand the very complicated photoionization with excitation cross sections. A jump to some of those systems, and there is a wide range of them, would be very interesting. One thing that was also discussed earlier in the meeting was the photoionization from excited states. I can only make a guess that one of the types of experiments that would be very interesting would be the ionization out of the low-lying excited states, not of the alkalis, but of the alkaline earths becasue you can predict that there will be tremendously strong resonance effects in those cross sections which would be amenable to calculation. I think that would be a nice match between theory and experiment.

B. CRASEMANN: These comments have shown, I think convincingly, convincingly to DOE too, I hope, what an enormous amount of really challenging work is waiting to be done with this facility.

WORKING GROUP SUMMARY

AREAS FOR STUDY AT NSLS

S. T. Manson

I. Three-Body Continuum Coulomb Problem - A central unsolved problem in physics. This needs in-depth study.

A. Double Photodetachment and Photoionization - Energy and angular correlation of continuum electrons from threshold to several hundred eV above needed; $h\nu + H^-$, He, O^-, F would be of great use; $h\nu$ dependence crucial.

B. Detachment (or Ionization) with Simultaneous Excitation - This leads up to the double ionization threshold. Needed are complete experiments, σ's, β's, spin polarization; H^-, noble gases (especially He), and alkaline earth elements are of greatest interest; $h\nu$ dependence crucial.

C. Highly Excited Autoionizing States - These mock up two electrons in the continuum (almost); H^-, noble gases (especially He), alkaline earths of interest; both absorption as well as the subsequent decay are of importance.

D. Threshold Auger (γ,2e) Experiments - This leads to a three-body continum Coulomb state; near threshold photo- and Auger electron interact, giving post-collision interaction; energy and angular correlation of ejected electrons needed as a function of $h\nu$ as $h\nu$ passes through the threshold. Inner shell photoionization of noble gases seems good here.

II. Open-Shell Atoms - Very little is known about their interactions; survey experiments desperately needed; relative cross sections okay

(where absolute too difficult), branching ratios, and β's are needed as a function of $h\nu$ from threshold; other than the alkalis (and a little on C, N, and O), there is just about no data on the open-shell atoms; particularly interesting are branching ratios for outer np photoionization in the halogen or chalcogen atoms, β's for the outer ns, np photoionization of the halogens Cl, Br, I, β's for the outer ns photoionization of Na, K, Rb, and Cs, and anything on very high Z.

III. Photoionization of Heavy (High-Z) Atoms - Very little is known; survey needed for σ, β, and branching ratios for $Z \geq 72$; particular attention to photoionization of outer (valence) and 5d electrons, and location of Cooper minima and partial cross sections; this will give us a handle on relativistic effects in photoionization. A particularly interesting case is atomic U if experiments are possible.

IV. Inner-Shell Spectroscopy - Particularly inner K and L-shells throughout the periodic system. Of special interest are experiments looking at K-shell photoionization of the first 100-200 eV above threshold with either electron spectroscopy of high resolution x-ray spectroscopy to isolate the satellite lines (ionization or excitation of a 1s plus excitation of an outer electron) from the normal line. Anything with $Z \geq 10$ would be of interest here, Cu particularly so.

V. Spectroscopy of Autoionizing States - As complete experiments as possible; isoelectronic sequences are of particular interest, e.g., Xe, Cs^{+}, Ba^{++} a particular favorite; spectroscopy of triple (and more) excited states, e.g., Li $2s^2 2p$, and other alkali and alkali earth elements might prove easiest.

VI. Ions - Virtually no data on photoionization, but significant data on optical oscillator strength exists.

A. Photoabsorption Cross Sections of Ions - Total and partial cross sections needed to test theory, O^{+n}, Fe^{+n} particularly interesting owing to applications to aeronomy and astrophysics.

B. Discrete Oscillator Strengths - Gives information complimentary to beam-foil excitation since one would look at absorption rather than emission. Of particular interest, Xe and Au isoelectronic sequences, in depth studies.

VII. Excited State Photoionization - Of interest owing to the huge physical size of excited states, survey data needed for σ and β as a function of $h\nu$. The alkali and alkali earth atoms are particularly amenable to such studies. In addition, inner shell photoionization of excited atoms should be of interest and there is no experimental data. Various new phenomena, e.g., multiple minima for Cs 5d, need experimental checks.

VIII. Molecules - Clearly a huge topic, only some high points will be mentioned; high resolution in depth experiments which distinguish vibrational states and elucidate the photoabsorption channels are needed; inner shell (K) data to elucidate the details of the shape resonance also required. This is really the province of molecular physics, but it impinges greatly upon atomic physics, and not enough was discussed at the workshop to make specific recommendations.

IX. Field Effects in Atomic Photoionization - Electric and magnetic fields (and both); high resolution spectroscopy needed with experiments done as a function of field strength; particular interest in the region around the ionization threshold(s).

WORKING GROUP SUMMARY

HARDWARE

T. Kruse

General Comments

Round table discussion indicated interest both in UV and in x-rays, and fell within three general affinity groups:

1) gas phase ("dense" targets),
2) beams and traps (tenuous targets),
3) instrumentation development (testing, calibration, materials).

Some desirable working features could include:

a calibration source of light - tracing the synchrotron optics, (possibly mounted at right angles with a mirror);

an insertable intensity monitor (possibly diode) to check grating degradation;

access to pumps, gauges, etc.;

information and perhaps a degree of standardization and cooperation concerning data acquisition, storage, software, (the NBS-NRL PRT has considered some of these questions).

Gas Phase

X-rays are of interest with nuclear type detectors

(eg, silicon).

In the UV, initial needs might be met as outside users on one of the presently planned lines, particularly U3 (BNL-Chemistry), which expects flux to 10^{14} sec^{-1} in 4 mm^2 with 77 mrad divergence, range 300-3000 A.U., normal incidence monochrometer, resolution about 50 millivolts at 20 ev.

The contact for U3 should be Mike White, BNL Chemistry. This PRT is large, with the usual 25% reserved for outside users. Hardware includes pumps, a versatile chamber, a molecular beam apparatus. Adaptation of specialized apparatus could be relatively inexpensive. Photo electron and photon spectroscopy should be possible.

The characteristics of other planned UV (ranging to 12000 AU) and x-ray lines can be found in Nuclear Instruments and Methods 172 (1980).

Ion Beams and Traps

The range and precision of experiments possible with these techniques is, in principle, very great. X-ray and UV are alike of interest. Modification of the state of the beam by tunable laser is possible and desirable (as for gas phase).

Rates begin to be adequate at the NSLS. Background could be a major problem, especially from interactions with residual gas particles. Very high vacuum may be necessary.

Storage ion traps need not be very expensive. It may be possible to extract electrons for analysis.

Development of sources of highly charged ions is under way in several countries. For singly charged (plus and minus) molecular and atomic ions, and for some doubly charged atomic ions, there are excellent commercial sources available.

Detection methods (ion, electron, photon) need consideration. For slow (kev) beams, time structure of the NSLS beam may not help much, in certain geometries. Photo-electron resolution by electron time of flight will necessarily anti-correlate with synchroton photon intensity (pulse repetition rate).

Instrumentation Development and Testing

The tunability, intensity, and known characteristics of the NSLS make it extremely attractive for calibration, testing, and development, to designers and users of instruments in other fields such as satellite astrophysics. Materials testing (reflectivity, longevity, etc.) might be very useful.

Conclusion

Evolutionary development of NSLS use for atomic physics seem practical and feasible, with need for time and special facilities clarifying as the facility develops. Techniques new to this range of photon energies begin to become possible

with present intensities.

If undulator sections become available in the future, their unique intensity characteristics would match beautifully the uniquely clean and controllable target characteristics of ion beam and storage devices.

CONCLUDING REMARKS

B. Crasemann
University of Oregon

I'll just take a minute because we are all played out. I think we have reason to be very grateful to Keith Jones and his colleagues on the Atomic Physics PRT, Brant Johnson, Don Gregory, Val Kostroun, and Ted Kruse, who have put this workshop together which has been a very stimulating experience for everybody. We have seen that there is really a wealth of important physics waiting to be done with synchrotron radiation, ranging up to the "perfect scattering experiment" of John Cooper's where "one goes differential in all parameters." Tom Carlson commented that "the best way to study many-body effects is by photoelectron spectrometry"; that may reflect his particular point of view but it is true --- XPS is a very powerful approach,and here people will have a chance to do this better than perhaps anywhere else. An important aspect mentioned only peripherally, when Daniel Lu brought it up, is the interface of atomic physics with other areas, from astrophysics to solid state to chemical physics; that is a very, very fertile area that might be explored more thoroughly in connection with the financial base of this enterprise, because many of those border areas or adjoining areas have such technological importance that it is easier sometimes to draw funding for them than for "pure" atomic physics.

I was very impressed with the concrete progress made, not only with the NSLS facility itself and the hardware we have seen, but with definite planning of such things as the ion transport systems and the gas-phase spectroscopy line on UV. Jerry Hastings and Malcolm Howells clearly are on the way to

designing superior monochromator and photon beam-handling systems. They are able to draw on the experience gained at other facilities and can incorporate improvements that will be extremely welcome. In the early days of synchrotron radiation experiments, some of you may have shared the experience of spending a long time sitting on the wrong reflection from a monochromator before realizing what is going on; with what is known now, your designers will surely be able to make the hardware so that users who are not specialists in that instrumentation can nevertheless operate it without too much special study of x-ray crystallography or whatever is involved. So one can be very optimistic that with this design being in such expert hands it will become really good.

When Eugen Merzbacher closed the x-ray conference in Scotland a couple of weeks ago, he quoted a famous French chef who had said "Whether one has eaten well one cannot tell until the following morning." This is a good quote to repeat here, I think. The following morning we will likely find that this workshop has brought together the people, some of whom didn't know each other at all before, who share an interest in atomic physics with synchrotron radiation, and that there will be a continuing interchange of ideas and continuing collaborations. Maybe that is as valuable a result of this effort as the fact that we shall have something really substantial to show to the funding agencies to give proof that there is important physics to be done here. So let me only once more say "thank you" to the organizers for their hospitality; we appreciate it very much.