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Report on the Workshop on New Directions in Soft X-Ray Near-Threshold Phenomena

Pacific Grove, CA
March 1–4, 1987

July 1988

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

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Report on the Workshop on New Directions in Soft X-ray Near-Threshold Phenomena

Asilomar Conference Center
Pacific Grove, CA
March 1-4, 1987

Sponsored by

Lawrence Livermore National Laboratory*
and
Lawrence Berkeley Laboratory†

Ingolf Lindau	Stanford Synchrotron Radiation Laboratory
Peter W. Langhoff	Indiana University
Richard H. Pratt	University of Pittsburgh
Manfred O. Krause	Oak Ridge National Laboratory
Carl L. Nordling	University of Uppsala
Richard L. Blake	Los Alamos National Laboratory

Edited by:

Dennis W. Lindle
Quantum Metrology Division
National Bureau of Standards
Gaithersburg, MD 20899

Rupert C.C. Perera†
Center for X-ray Optics
Lawrence Berkeley Laboratory
University of California
Berkeley, CA 94720

Supported under U.S. Department of Energy Contract Numbers
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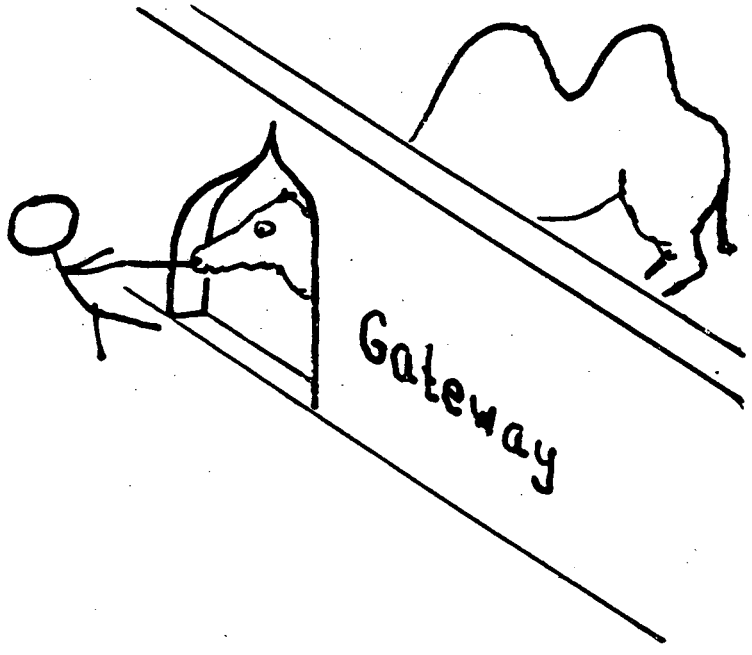
Gateway

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I. Introduction

The "Workshop on New Directions in Soft X-Ray Near-Threshold Phenomena" was held at the Asilomar Conference Center in Pacific Grove, CA on March 1-4, 1987. It was attended by 59 scientists from 8 countries, representing 27 institutions. Major funding for the meeting was donated by L-Division of the Lawrence Livermore National Laboratory, who hosted and organized two previous workshops on photoabsorption and scattering in the soft x-ray energy range. Additional funding was provided by the User's Group of the Advanced Light Source.

The Workshop, as its name suggests, emphasized physical phenomena in atoms, molecules, and solids near inner-shell thresholds. Of particular interest were threshold ionization, post-collisional interaction, resonant photoemission and fluorescence, and multi-electron effects such as shake-up and shake-off. In these areas and others, special consideration was given to presenting recent discoveries and potential "new directions" for future work. The agenda of the Workshop is reproduced in Appendix I.

A diverse group of experimentalists and theoreticians attended the Workshop and many of the world's experts on inner-shell phenomena participated. While the techniques and perspectives of the participants were quite varied, all were drawn together by a shared interest in near-threshold effects. The meeting was timely in that much new and interesting work has been produced recently, with tantalizing expectations for the future.

The Program Committee, chaired by Richard Pratt of the University of Pittsburgh and the Organizing Committee, co-chaired by Dennis Lindle of the National Bureau of Standards and Rupert Perera of Lawrence Berkeley Laboratory, were responsible for the technical program, as well as for arrangements at the meeting site. A full listing of the members of these two committees is included in Appendix II.

II. Session 2a: Photoabsorption

Ingolf Lindau

C.E. Brion reported on a compilation of absolute total photoabsorption and partial-channel photoionization cross sections for the valence shells of selected molecules, including diatomics (H_2, N_2, O_2, CO, and NO), triatomics (CO_2 and N_2O), simple hydrides (H_2O, NH_3, and CH_4), hydrogen halides (HF, HCL, HBr, and HI), sulfur-containing compounds (H_2S, CS_2, OCS, SO_2, SF_6), and chlorine-containing compounds (Cl_2 and CCl_4). The partial-channel cross sections presented refer to production of individual molecular ionic states to electronic resolution, and also to production of parent and specific fragment ions, as functions of incident photon energy, typically from ~10 to 100 eV. It was stated that absolute photoabsorption cross sections are in all cases considered to be better than 10% and, in many cases, better than 5% (for the diatomic and triatomic molecules). Total photoabsorption cross sections above the first ionization threshold are reported from conventional optical measurements obtained using line sources and continuum synchrotron radiation, and from "equivalent-photon" dipole (e,e) electron-scattering experiments. Partial photoionization cross sections for production of electronic states of molecular ions are obtained from photoelectron spectroscopy and from dipole (e,2e) coincidence measurements. Photoionization mass spectrometry and dipole (e,e+ion) coincidence studies provide measurements of partial cross sections for ionic photofragmentation (i.e., molecular and dissociative photoionization). Photoelectron anisotropy factors, which together with electronic partials, provide cross sections differential in photon energy and ejection angle, also are reported. There is good agreement between cross sections measured by the physically distinct optical and dipole electron-impact methods. The cross sections and anisotropy factors also compare favorably with selected ab-initio and model-potential (X-alpha) calculations, largely in one-electron approximations, which provide a basis for interpretation of the measurements. A final comment was that the compilation will be published in J. Phys. Chem. Ref. Data, but there is still time to provide input to the data base (at the time of the Workshop).

E.E. Koch reported that near-edge extended x-ray absorption fine structure (NEXAFS) and shape resonances have been observed for a number of condensed molecules and adsorbates in different types of experiments. As pointed out by Dehmer et al., one basically expects the same set of resonances shifted in energy depending on the type of experiment: (i) in core-hole-excited absorption there is a strong Coulomb attraction, so the resonances are pulled down relative to the vacuum level; (ii) by

carefully measuring the partial valence-shell photoemission cross sections one can map out the density of final states and thereby locate the resonances in the partial cross sections; and (iii) finally, in electron scattering and inverse photoemission the same set of resonances can be observed, now shifted further up into the continuum by the Coulomb repulsion between the electron in the resonance state and the neutral molecule. This situation is illustrated by solid SF_6, a case with strongly localized resonances, and for solid N_2 and CO_2 where one observes S band formation (overlap of final states on neighboring molecules). New experimental C 1s excitation spectra for condensed aromatic hydrocarbons oriented on single-crystal surfaces and Langmuir-Blodgett films also were discussed. They show pronounced polarization dependence and a detailed fine structure in the range of C 1s $\rightarrow \pi^*$ excitations which can be explained satisfactorily by calculations and comparison to electron-scattering data. Brief comments were made concerning the nature of the σ resonances in benzene and Langmuir-Blodgett films.

C. Bonelle focussed on excited-state resonant emission and the characteristics of absorption and reflection spectra when resonance lines are present, and pointed out that resonant emission is a transition which takes place in an excited atom and corresponds to the return of the excited electron to its hole. Thus, the x-ray resonant state is an excited state with a hole in a core level which may decay by the return of the excited electron, the excess energy coming off as a photon or as an electron. These phenomena were illustrated by Gd, Dy, and La 3d spectra, and a detailed comparison between the reflected and transmitted intensity spectra of La in the 3d threshold region was made. Two strong maxima in the reflected intensity were observed, slightly shifted with respect to the two absorption lines. This behavior is characteristic of the presence of quasi-atomic resonances in the cross-section variation. The scattering factor is strongly dependent on the resonant term, and thus it is important to determine the contribution of the scattering to the shape of the photoexcitation spectra. Some model calculatons were presented based on the data tabulated by Cromer and Liberman. The real part of the scattering factor introduces an asymmetry towards higher energies of the scattering cross section. The energy dependence of the total cross section can thus be asymmetrical and the photoexcitation cross section symmetrical. Because the cross section has a quadratic dependence on the scattering factor, the conclusion was that the photoexcitation lines must be described in the framework of scattering theory.

N. Kerr Del Grande reported on synchrotron-radiation measurements of near-threshold and broad-range (80-1000 eV) absolute photoabsorption cross sections taken using the plane-grating monochromator on beamline U14A at the National Synchrotron Light Source. Transmisson data for well-characterized multilayer foils of C, Ti, Cr, Ni, Cu, Th, and U

Sessions 2b and 3: Photoionization

Peter W. Langhoff

A central theme of the Workshop was the notion that core states in photoabsorption can be prepared in various configurations (M^* vs M^+) by incident-photon-energy selection, with the subsequent decay dynamics by photon or electron emission and ultimately dissociation dependent upon this preparation. The changing decay dynamics with incident photon energy manifests itself in differing fluorescence and/or Auger and autoionization energy spectra, which require theoretical and computational interpretation to clarify the underlying dynamical events.

Good progress was reported at the Workshop on experimental aspects of the variations of fluorescence spectra, including different polarizations, with incident photon energy near edges, and in corresponding "resonance" Auger spectra. In the latter case, post-collisional interaction (PCI) between Auger and photoemission channels have now been studied carefully. Continuing interest attaches also to shape resonances in inner-shell partial cross sections, particularly in satellite channels, in which cases both collapse times into shake-up and shake-off ionic states and the Wigner delay time associated with the resonance are involved. Possible coupling between satellite and main-hole channels may also be involved. These data, as well as the growing number of Auger and photoemission studies reported under differing resonance excitation conditions in molecules, require clarifying theoretical interpretation. The molecular ionic fragmentation patterns following near-edge excitation and electron emission decay studied by coincidence techniques described at the Workshop would seem to follow the complete range of time scales in soft x-ray molecular photoprocesses, and provide a challenge for complete theoretical conceptual interpretation.

Progress was reported in these sessions on theoretical and experimental aspects of PCI, with particular reference to K-shell cross sections and Auger line shifts and shapes by T. Åberg and V. Schmidt. Continuing his earlier remarks on theoretical descriptions of fluorescence and Auger decay made in Session 1, Åberg emphasized the dominant role played by screening in the final (two-electron) channel in accounting for observed Auger line shifts and shapes. Schmidt reported experimental measurements of the shift and shape of the $4d^{-1} \rightarrow 5p^{-2}$ Auger line in Xe, and on interpretations based on semi-classical models, with particular emphasis on the vanishing of PCI in the case of sufficiently large excess photoelectron kinetic energy (the "no passing" effect). Descriptive accounts are provided herewith of these contributions.

It will be recalled, PCI refers to the interaction between outgoing Auger and photoelectrons, which can be particularly important for low

photoejection kinetic energy (near threshold), in which case the Auger electron can overtake and interact strongly with the photoelectron. Åberg's theoretical description of the event is based on multichannel scattering theory in which the Auger effect arises as a resonance in the double photoionization channel. This particular approach incorporates preconceived notions regarding time scales, but nevertheless gives a picture of the Auger effect largely in accord with that of diagrammatic and semi-classical methods. In particular, when a screened Coulomb potential is used in the final channel, there results an Auger line shape in precise accord with semi-classical results and experimental values. With reference to the corresponding (K-shell) cross section, PCI apparently provides a very small correction to relaxed-core calculations, although there may be a more significant effect upon frozen-core calculations. Further developments in theoretical treatments of PCI will include a merging of the scattering-theory approach with time-scale concepts and possible simplification and clarification of the computational steps involved in obtaining detailed results.

Schmidt's measurements of Auger line-center shifts as a function of excess (photoelectron) kinetic energy demonstrated clearly the vanishing of PCI above the "no passing" photoelectron energy, and gave line shapes in excellent accord with semi-classical and scattering-theory calculations in the case of $4d^{-1} \rightarrow 5p^{-2}$ in Xe. Since the Auger shifts are small (~ 0.1 eV) even at the lowest kinetic energy achieved, monochromator and analyzer bandwidths and related data interpretation require careful consideration. The semi-classical approaches to shifts and shapes provide a particularly clear basis for interpretation of the measured values including the appropriate shift values. Continuing studies in this area will explore PCI as a link between inner-shell ionization and excitation processes, relations between PCI shifts and inner-shell level widths, emission-angle-dependent PCI, and possibly, consequences of angular-momentum exchange in the final two-electron Auger channel.

Following the presentations on PCI, progress was reported by five experimental and one theoretical worker in the area of near-edge photoionization processes with emphasis on Auger spectral shifts, molecular fragmentation following excitation, and satellite photoemission and partial cross sections in various forms.

T.A. Carlson reported some of the first angle-resolved photoelectron-spectroscopy measurements for excitations below the Si, S, and Cl 2p edges in CS_2, OCS, $SiCl_4$, and chloromethanes. Auger and valence-shell photoemission due to hole-state autoionization (see Fig. 3-1) are disentangled employing the apparent high β values associated with the latter. In this way Auger shifts are measured for specific lines, which values correlate well with a simple spectator model for the pre-edge excited electron employing Bohr-atom notions.

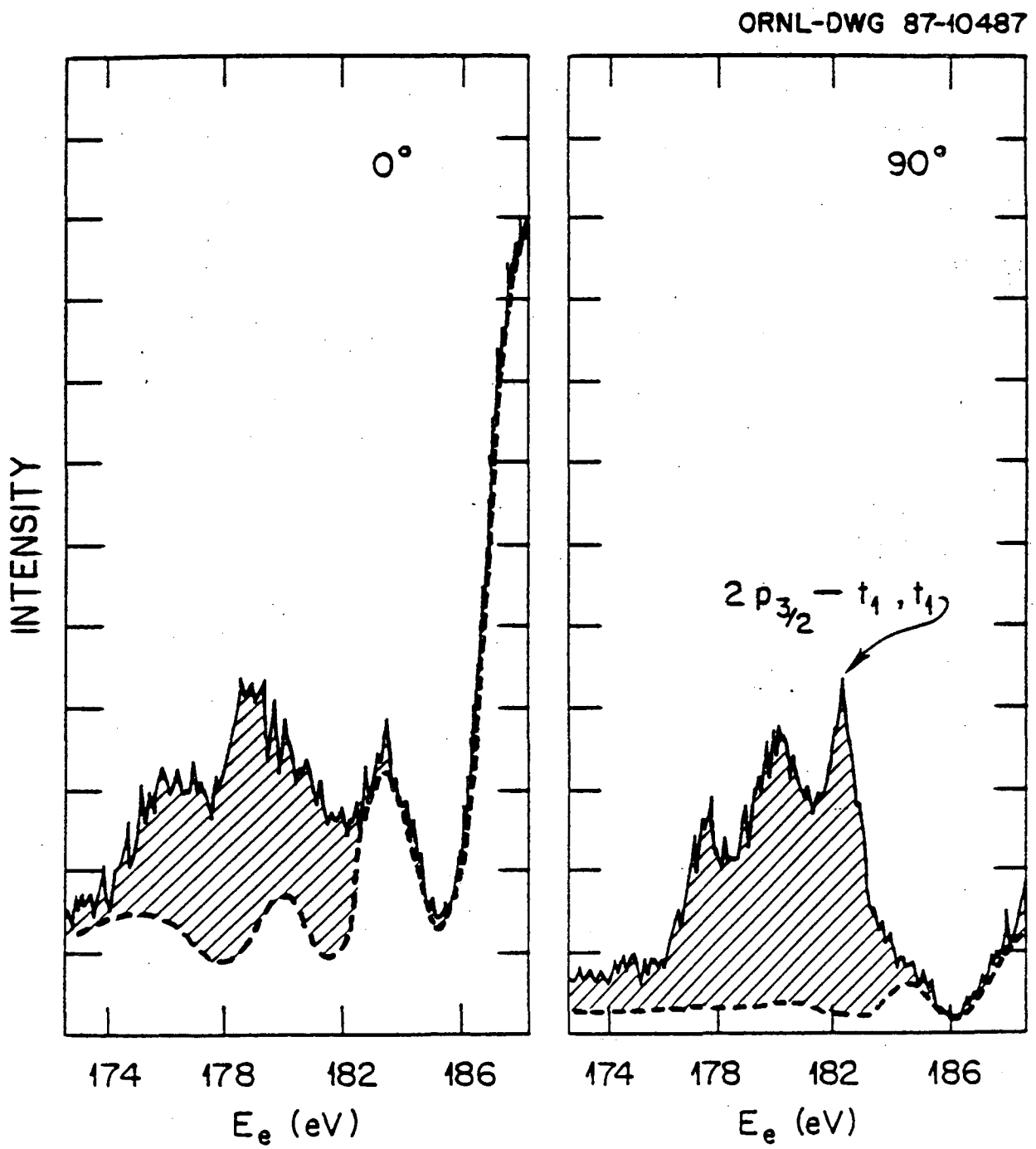

Figure 3-1. Electron spectra from the first preionization in CCl_4 near the Cl 2p edge. The clear areas represent contributions from the photoelectron spectra of the valence shell; the striped areas are the Auger spectra.

G.M. Bancroft reported studies on Si 2s and Si 2p absorption-edge structures in $SiCl_4$, corresponding resonance valence-shell Auger spectra as a function of exciting light, related resonance studies of Ar lines (see Fig. 3-2), and both experimental and computational (Xα) studies of the valence shells of SF_6 and SeF_6. The observed Auger lines in both $SiCl_4$ and Ar are seen to exhibit intensity variation with exciting (resonant) light, in accordance with production of different initial states for the subsequent decay. Calculations on an F_6 cage in the absence of a central sulfur atom attribute the origin of a high-energy resonance (60 eV kinetic energy) in the valence partial cross sections to F atoms rather than to the sulfur e_g and t_{2g} orbitals.

W. Eberhardt reported on Auger decay and subsequent ionic fragmentaton following K-edge excitation in N, C, and O containing molecules, with particular reference to N_2 and CO. Vibrational structures in the electron spectra are in accord with Franck-Condon effects in the associated potential curves. Possible interference effects are inferred from the differences between the absorption and emission processes in these experiments.

Threshold photoemission and partial-cross-section measurements were reported by T.A. Ferrett, with particular emphasis on multielectron processes in inner-shell photoionization (see Fig. 3-3). Strong resonant shake-off was observed in $Ar(2p^{-1})$, $Kr(3d^{-1})$, and $Xe(4d^{-1})$, threshold spectra, and multielectron character inferred from resonance features in $S(2p^{-1})$ satellite partial channels of SF_6.

Further details of $Ar(3s^{-1})$ and $Xe(5s^{-1})$ satellite photoemission were reported by C.E. Brion using photon techniques (see Fig. 3-4). These provide a basis for reinterpretation of earlier (e,2e) measurements of these features, in which cases good agreement now exists between experiment and calculated spectroscopic factors.

Aspects of Xα photoionization calculations, particularly on $SiCl_4$ $Si(2p^{-1})$ shape-resonance channels (see Fig. 3-5), were reported by F. Grimm. These studies show a number of strong post-edge features which are fully characterized by the calculations. An attempted correlation between Xα and minimal-basis-set orbital calculations on C_6H_6 achieved only a partial correlation of shape resonances with orbital positions, suggesting that further clarifying studies are in order.

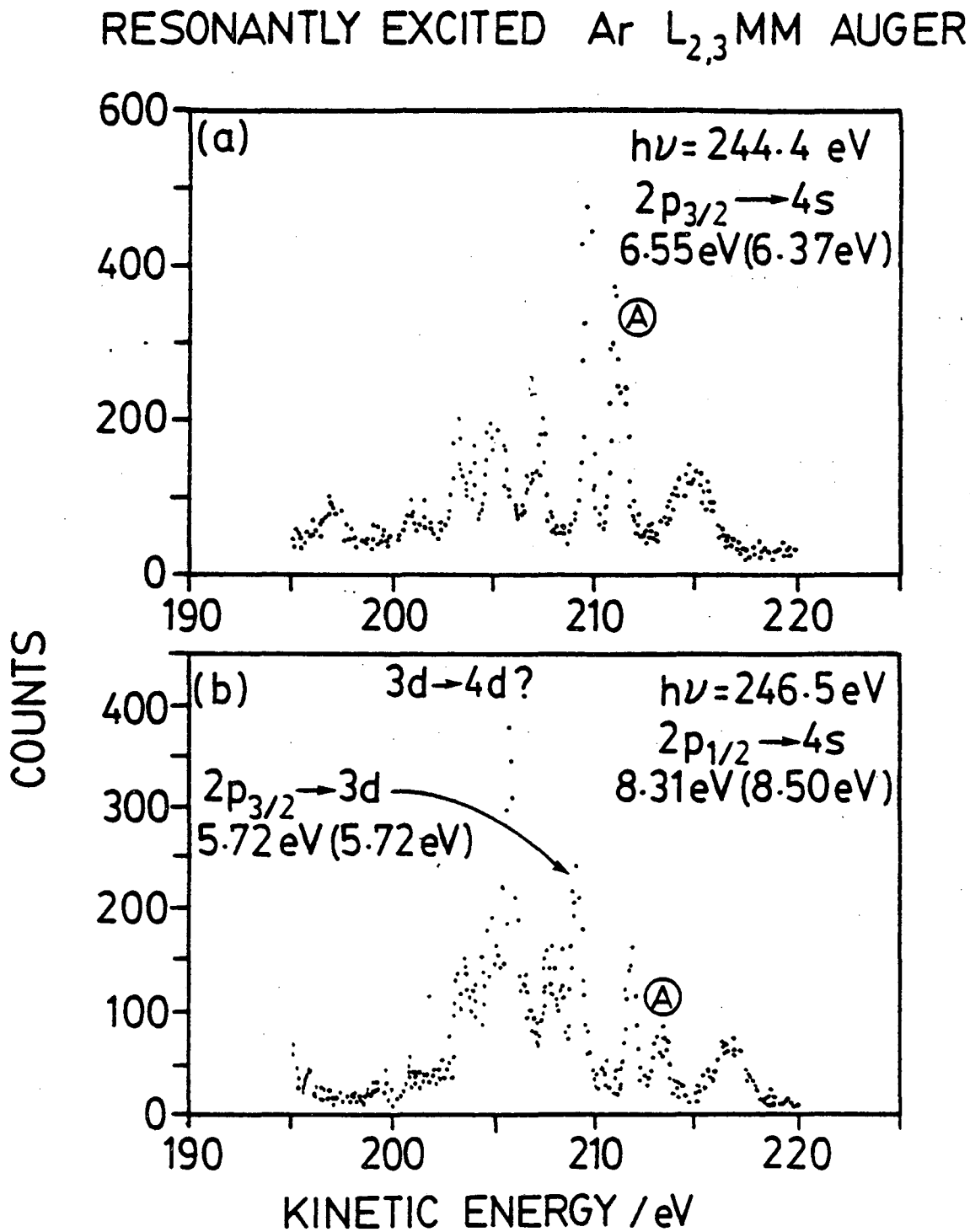

Figure 3-2. Resonant photoemission spectra from Ar.

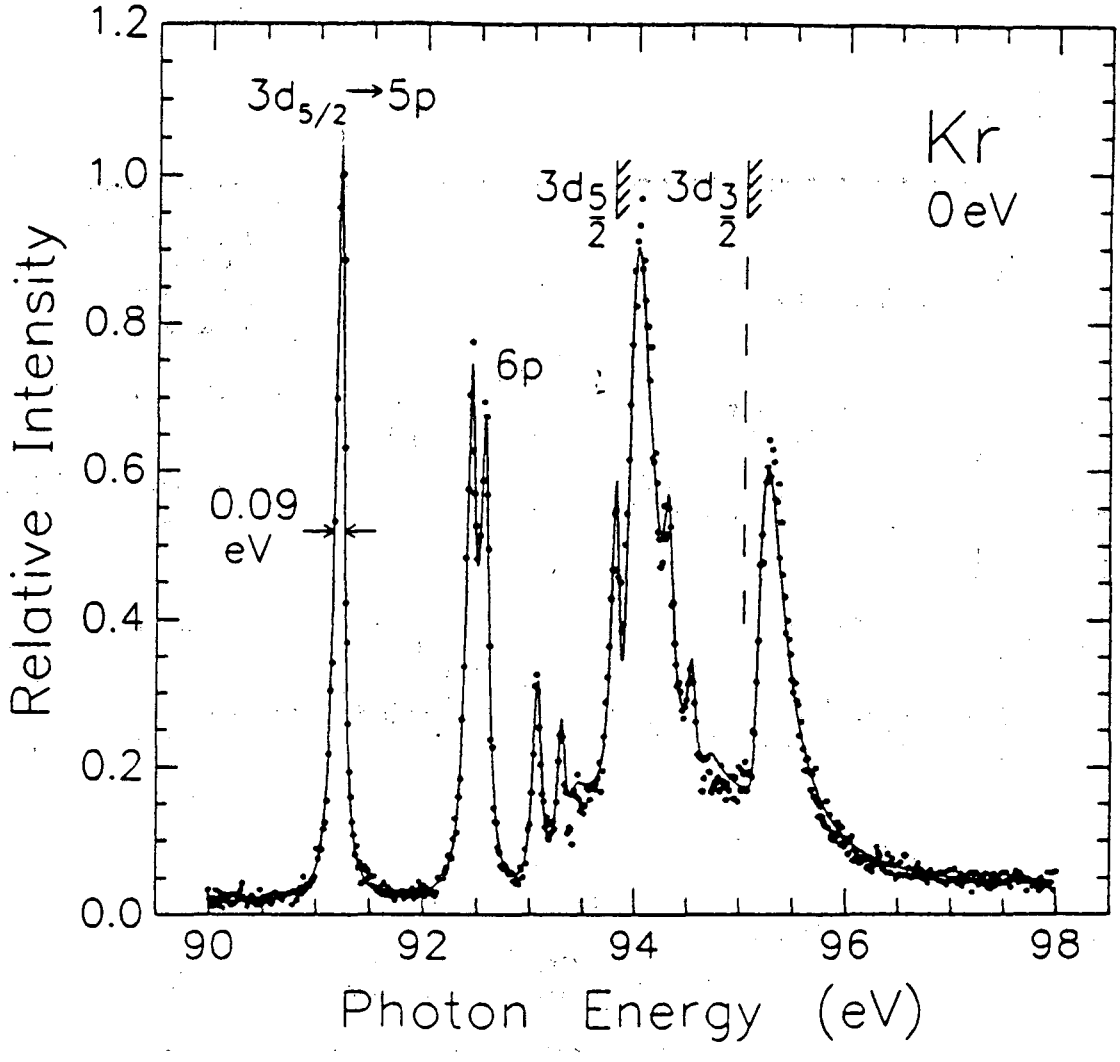

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Figure 3-3. Threshold electron spectrum of Kr near the 3d edge.

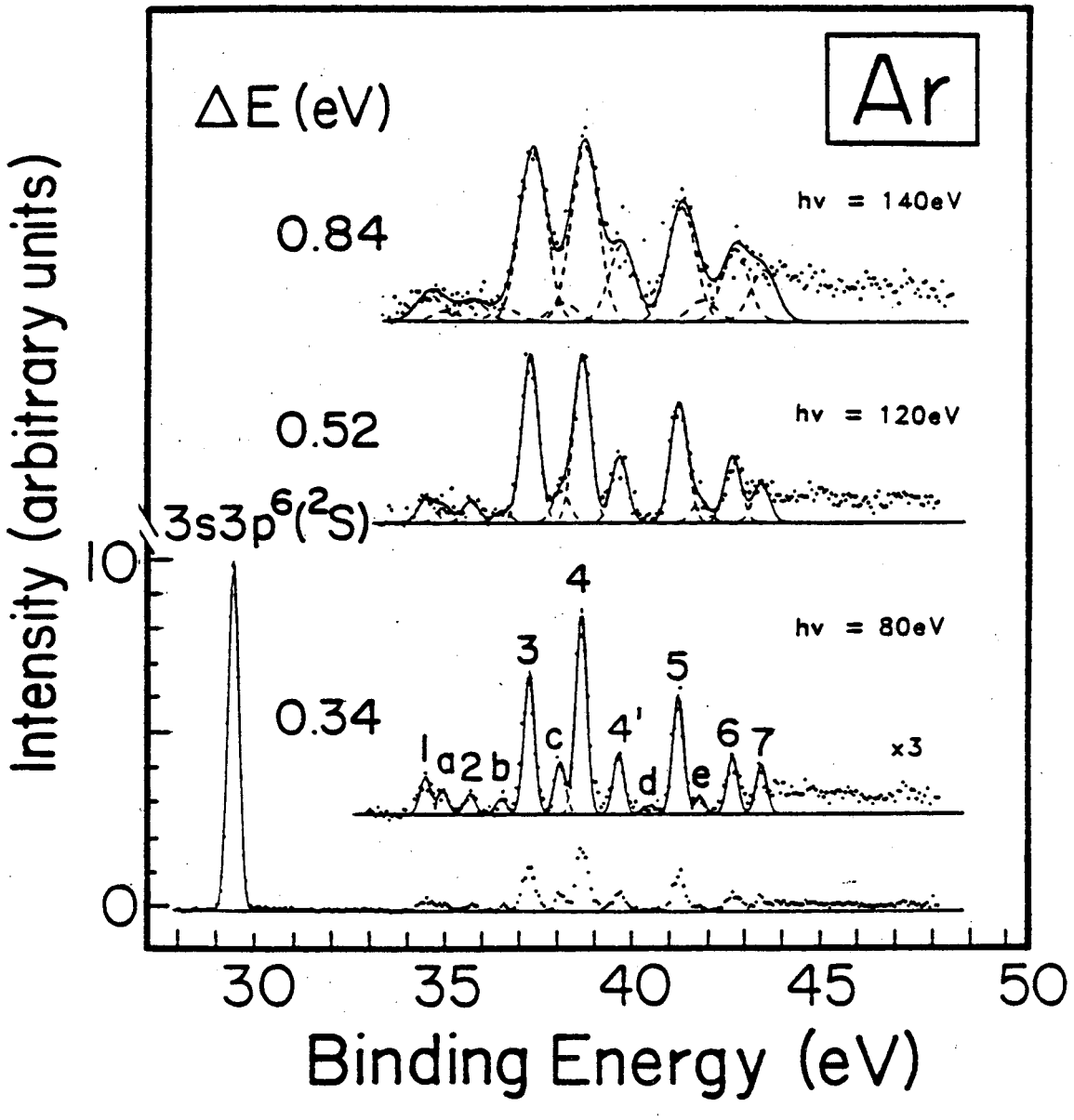


Figure 3-4. Ar $3s^{-1}$ photoelectron satellites.

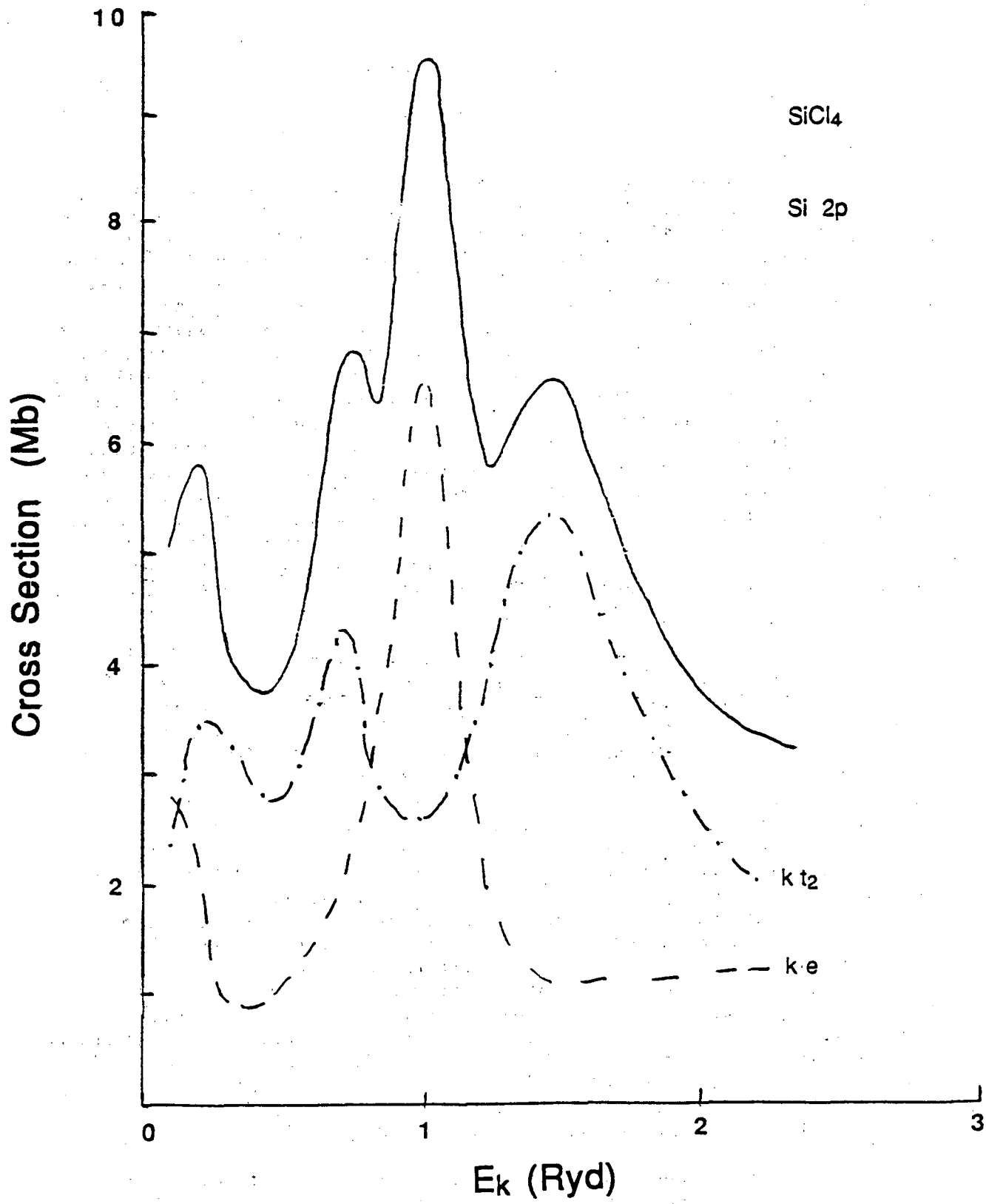


Figure 3-5. MSM Xα calculation of the Si 2p cross section of $SiCl_4$.

IV. Session 4: Theory

Richard H. Pratt

In this session, the general status of photoabsorption theory was reveiwed by A.F. Starace, and the corresponding status of elastic photon-atom scattering theory was reviewed by L. Kissel. As an introduction, D. Smith reviewed the dispersion relations which connect these two processes, and the related sum rules (see Figs. 4-1 and 4-2). These relations constrain data sets (whether experimental or theoretical) and can be used to judge consistency. Both Smith and Kissel pointed out that in the pioneering tables of Cromer and Liberman f′ was determined through dispersion relations from photoabsorption, but using an incorrect high-energy-limit value. This leads to an energy-independent Z-dependent correction which becomes large in high-Z elements and explains discrepancies reported by experimentalists (see Figs. 4-3 and 4-4). The relativistic high-energy-limit correction is apparently first identifiable in the work of Franz, and was calculated in special cases by Levinger (photoabsorption), and by Goldberger and Low, and Gavrila and Florescu (scattering); it can be confirmed in the numerical calculations of Kissel. A proof that the modified form factor (mff) approximation of Franz gives the correct high-energy limit for forward scattering is still needed. Corresponding useful relations for finite angle (or finite momentum transfer) are not known.

The theory of photoabsorption or scattering begins with the independent-particle approximation (IPA), which is simple-minded and inclusive (i.e., to sum over all processes consistent with the observed variables). Often it is an advantage to be inclusive. The simple-minded aspects of the IPA are most appropriate at high energies, but much less so in the edge regions which were the focus of this Workshop. But the IPA does provide a qualitative understanding of these two processes even near threshold. In photoeffect, beyond the basic features already present in a point Coulomb potential, screening of the central potential leads to two new features: shape resonances (corresponding to resonances in potential scattering when the potential has a barrier partially isolating an inner well) and Cooper minima (where dominant matrix elements change sign, considered as a function of energy, and cross sections are small). The corresponding understanding of the scattering problem is represented by the resonance and edge structure of the point Coulomb calculation, together with form-factor approximation for the inclusion of retardation effects. There are significant relativistic modifications to potentials and to the processes, which also can be understood at the IPA level. Substantial IPA data for photoeffect have been available for some time. It has recently become available for scattering (see Fig. 4-5), and when combined with knowledge of edge positions can yield quite good agreement with x-ray scattering experiments (see Fig. 4-6).

For a quantitative description of these processes in the near-threshold region, however, it is necessary to go beyond the IPA and include at least

Alternative Dispersion Relations

X-Ray form

$$f_1(\omega,0) = f_1(\infty,0) - \frac{2}{\pi}\mathrm{P}\int_0^\infty \frac{\omega' f_2(\omega',0)}{\omega'^2-\omega^2}d\omega' \quad \text{(A)}$$

- Fixed for $\omega = \infty$ at $f_1(\infty,0)$ Therefore, best at high energy.

Optical form

Use fact: no scattering by bound electrons at $\omega = 0$

$$f_1(0,0) = 0 \longrightarrow f_1(\infty,0) = \frac{2}{\pi}\int_0^\infty \frac{f_2(\omega',0)}{\omega'}d\omega'$$

substitute in (A)

$$f_1(\omega,0) = -\frac{2\omega^2}{\pi}\mathrm{P}\int_0^\infty \frac{f_2(\omega',0)}{\omega'(\omega'^2-\omega^2)}d\omega' \quad \text{(B)}$$

- Fixed for $\omega = 0$ at $f_1(0,0) = 0$. Therefore, best at low energy.
- Equivalent to an old friend from "optics 1"

$$n(\omega) = 1 + \frac{2}{\pi}\mathrm{P}\int_0^\infty \frac{\omega'\mathrm{K}(\omega')}{\omega'^2-\omega^2}d\omega'$$

Figure 4-1. Alternative dispersion relations.

T-R-K "f" Sum rule (non-relativistic)

from $f_1(\omega = 0, 0) = 0$ we found

$$f_1(\infty, 0) = \frac{2}{\pi}\int_0^\infty \frac{f_2(\omega, 0)}{\omega} d\omega$$

by Optical Theorem $f_2 \longleftrightarrow \sigma$

$$f_1(\infty, 0) = \frac{\mathrm{mc}}{2\pi^2 \mathrm{e}^2}\int_0^\infty \sigma(\omega) d\omega$$

so by T-R-K sum rule

$$f_1(\infty, 0) = Z = \frac{\mathrm{mc}}{2\pi^2 \mathrm{e}^2}\int_0^\infty \sigma(\omega) d\omega$$

Answer to dispersion relation conflict —

X-Ray and Optical forms equivalent only if experimental data verifies the T-R-K sum rule. That is, *all the absorbtion must be there.*

Figure 4-2. T-R-K "f" Sum Rule (nonrelativistic).

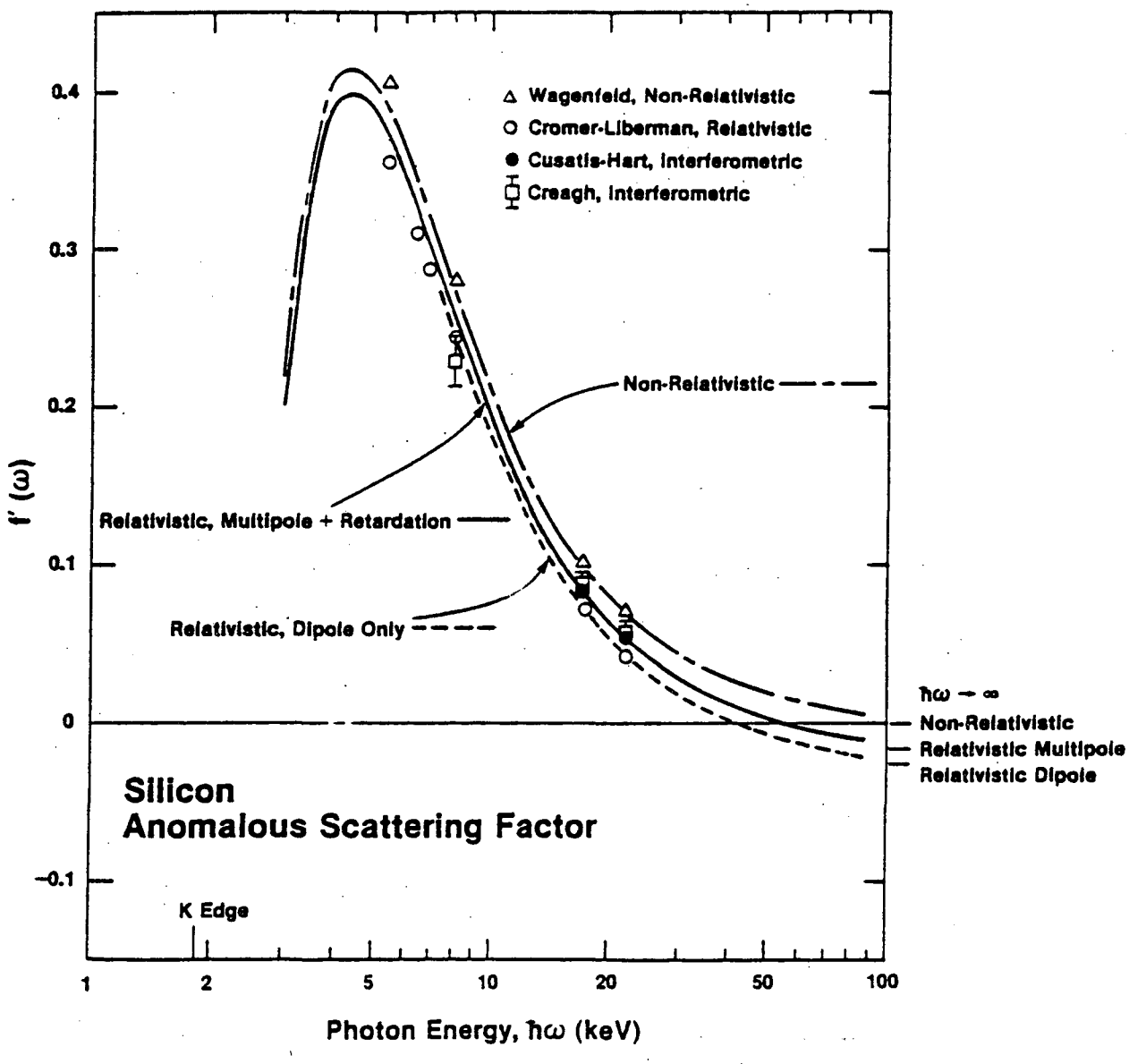


Figure 4-3. Silicon Anomalous Scattering Factor.

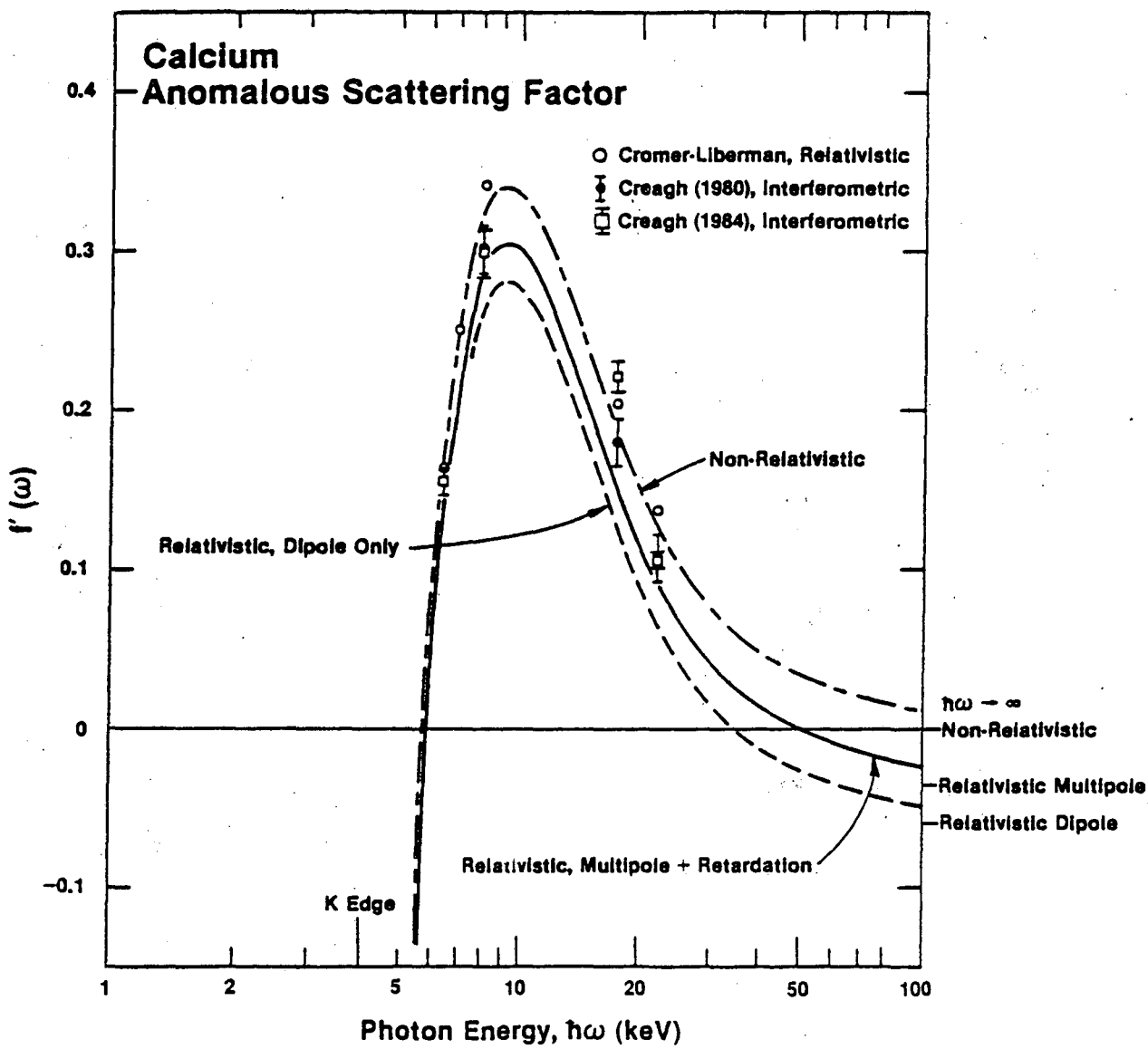


Figure 4-4. Calcium Anomalous Scattering Factor.

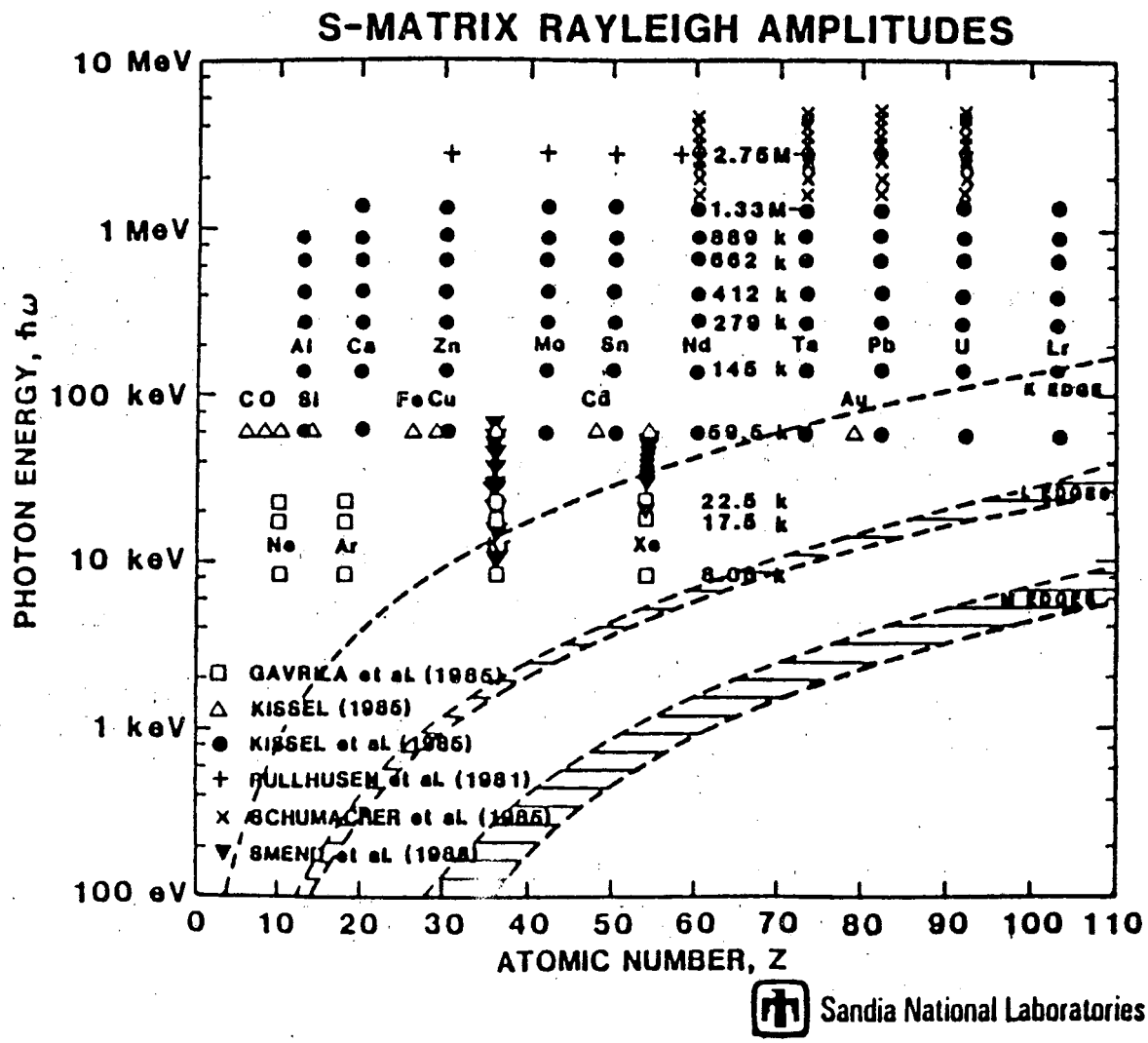


Figure 4-5. S-Matrix Rayleigh Amplitude.

NEAR XE K EDGE

- S-Matrix Approach
  K edge binding 34.56 keV
  photon energy 34.26 keV (0.3 keV below edge)

$d\sigma/d\Omega$ (r_0^2/sr)

angle	SM-KS	SM-KS'	SM-KS''	SM-S	experiment
0	2290	2450	2500	2500	
60	33.7	50.2	58.2	58.7	60.2 (2.9)
90	3.53	9.04	12.4	12.5	12.2 (0.7)
120	0.279	3.44	4.96	4.99	4.8 (0.3)
180	0.749	1.02	3.29	3.28	

SM-KS => S-matrix approach, Kohn-Sham exchange
SM-KS' => S-matrix approach, Kohn-Sham exchange, truncation correction
SM-KS'' => S-matrix approach, Kohn-Sham exchange, energy shifted
SM-S => S-matrix approach, Slater exchange
experiment => Smend et al (1987) - averaged over photon polarizations

lk 3/87

Figure 4-6. Near Xe K Edge.

some aspects of the electron-electron correlations (see Fig. 4-7). Such calculations (at TDLDA, RRPA, or MBPT levels) can be quite sophisticated; they tend also to be more exclusive in their description of reactions, which can be a disadvantage. For photoeffect, such calculations are now quite generally available and, as Starace described, in most cases good agreement with experiment has been achieved. However, one does not have systematic tabulation of photoeffect cross sections at this level of sophistication. For scattering, calculations including correlation effects are generally not available, and indeed have not been formulated.

The situation for photoeffect is not as good as the above statement may suggest. One problem, as discussed by D.A. Shirley in Session 1, is that additional excitation and ionization often accompanies the basic process. If not distinguished experimentally, it must be included in the calculation, which beyond the IPA can require separate (and sometimes more difficult) calculations. Another problem, noted by S.T. Manson in Session 5, arises when there are three (or more) charged particles in the final state (as in double photoionization). The appropriate boundary conditions for the three-body problem with long-range forces are not known. Still another problem, discussed by T. Aberg in Session 1, arises from the characterization of the final states of these processes. We think of photoeffect, perhaps followed by fluorescence or Auger emission, as two separate processes distinguished in time, and different from the single process of Compton scattering. But the time scales can be such that this distinction is blurred and hence a unified theory, such as Aberg discussed, is needed.

So far we have discussed those two processes in the context of an isolated neutral atom. But we have heard at this Workshop about the interest and importance of other situations. Even at the IPA levels there are new features for molecules, for example, associated with the non-spherically symmetric potential. Further changes occur as we proceed toward solids and levels broaden into bands. Even in the isolated-atom case, as Manson has noted, simple theory predicts significant changes for excited states and for ions, and experiments are awaited. Other environments also modify these processes, as in hot dense plasmas or high magnetic or electric fields.

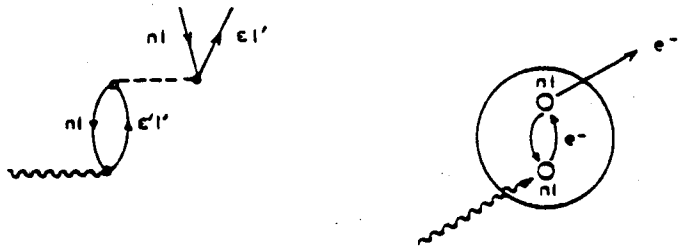
Finally, we should not be parochial in restricting our attention to these particular two processes: the photoeffect and scattering. Other processes test the same phenomena and give us further information. One example is provided by electron-initiated processes, as discussed by G. Wendin. It is well known that free-free transitions, for a near-threshold final continuum electron, sample situations which are also of concern in the bound-free transitions. Calculations exist at the IPA level, and Wendin discussed their extension to the circumstances in which correlations are important. This may be compared with the "atomic" bremsstrahlung discussed by Amusia. Finally, we heard from Y. Ohmura on the calculation of the Compton process, which Aberg had discussed as the fusion of photoeffect and fluorescence. We do not yet have a convincing IPA calculation of Compton scattering from atoms that goes beyond the standard incoherent scattering-factor approximation. Ohmura addressed modifications which must be considered in the solid, illustrated by structure found near the Cu K edge (see Figs. 4-8 and 4-9). But in either case it is clear that further experimental insight is available if a suitable theoretical calculation can be performed.

ELECTRON CORRELATIONS: PARTICLE-HOLE INTERACTIONS

(a) Intrachannel Interactions

-Very Large for Closed Shells

-Included in $V^{N-1}(LS)$ HF basis

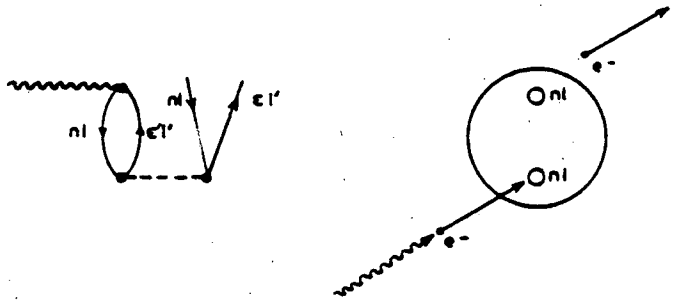


(a)

(b) Ground State Correlations

-Implies More Diffuse Atom

-Weakens Effect of Intra-channel Interactions



(b)

(c) Interchannel Interactions

-Important for Weak Channels

-Necessary to Describe Resonances

(c)

MBPT diagrams (left) and scattering pictures (right) for the following interactions: (a) intrachannel scattering following photoabsorption; (b) photoabsorption by a virtual doubly-excited state of the atom; (c) interchannel scattering following photoabsorption.

Figure 4-7. Electron Correlations: Particle-Hole Interactions.

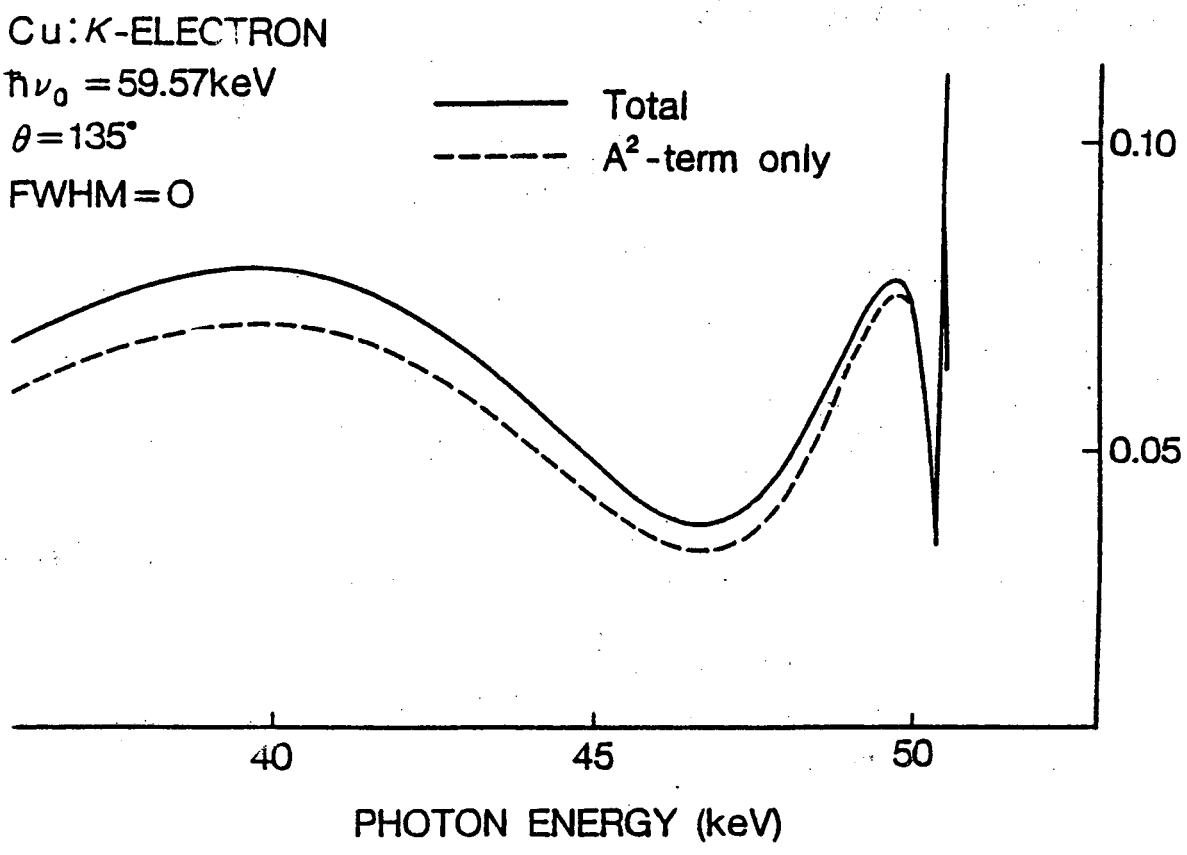
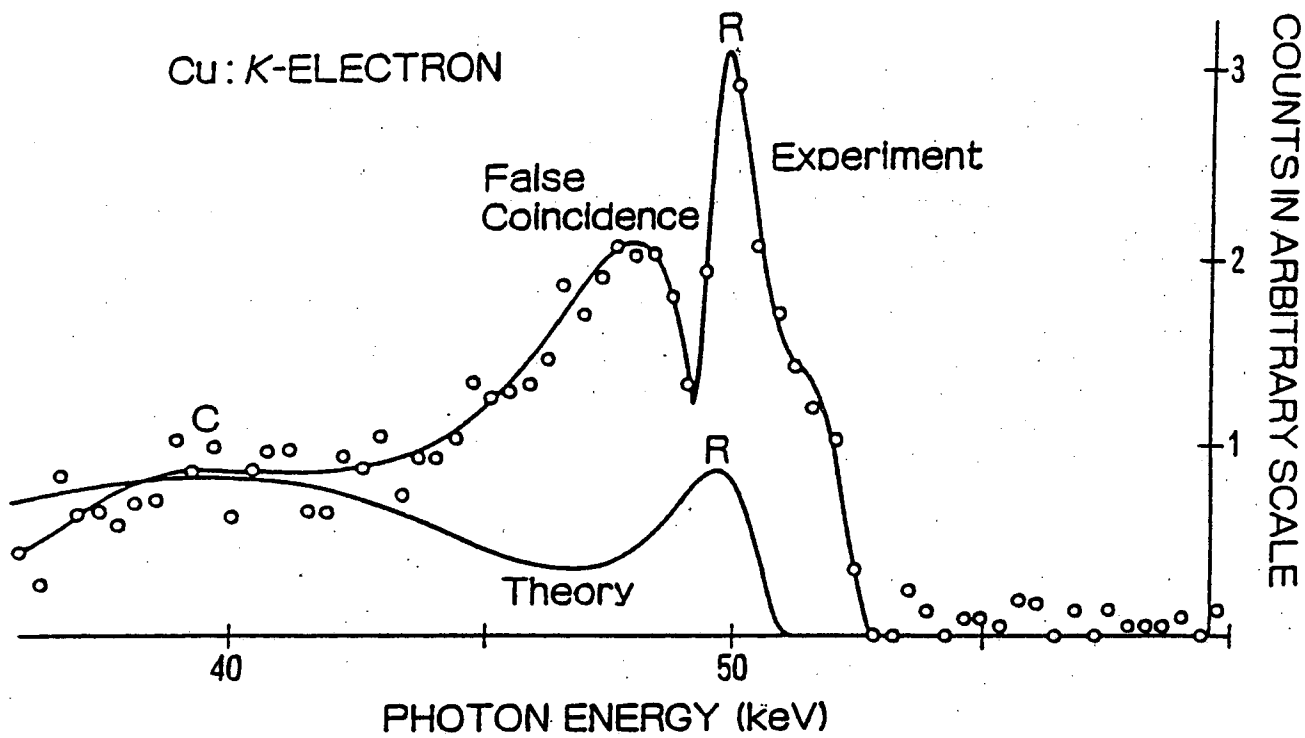


Figure 4-8. Inelastic scattering of gamma rays by Xu-K-shell electrons.



Solid line "theory" is spectra obtained by the present study. Solid line "experiment" is spectra obtained experimentally by Namikawa and Hosoya.

Figure 4-9. Spectrum from Fig. 4-8 corrected by p.A. terms.

V. Session 5 -- Future Capabilities Offered by Advanced Synchrotron-Radiation Sources

Manfred O. Krause

Virtually all the experimental work discussed at the accompanying workshop involves the use of SR. It is therefore only natural that the atomic and molecular physics community is thinking of future sources of this nature with better performance characteristics than the present sources, and about the opportunities offered by advanced designs.

The conclusions reached at the Berkeley workshop on an advanced SR source in November 1985 were reinforced by the presentations in this symposium. In fact, that we were emphasizing threshold phenomena at this meeting accentuated some of the most important points. They are, in terms of photon-source performance parameters: (1) high resolution, which should be better than 0.005 Å in the 10 to 100 eV range, and better than the natural atomic-level width at higher energies, namely less than 1 part in 10^4; (2) a healthy flux of at least 10^{10} photons/s at this resolution, and preferably much higher; (3) a strong flux of circularly polarized radiation which is not substantially smaller than that of the linearly polarized radiation; and (4) a time structure on the order of picoseconds or better. The resolution/flux requirements translate into a very low emittance beam due to monochromator characteristics and the need for a small source size for the high-resolution systems used in the analysis of the final photoproducts.

The characteristics summarized above are those considered universally important by the community of SR users involved in atomic and molecular physics. Other characteristics of advanced SR sources may be useful for specific experiments that are not dealt with in this report. Accordingly, the following discussion assumes that improving the flux/resolution parameters of a SR source will produce initially the most significant new results in atomic and molecular physics. This is not to say that other improvements, such as in-time structure or providing a source of circularly polarized radiation, are not useful, but this report recognizes that the SR community is so "flux-" and "resolution-starved" that the first major gains will come with flux and resolution enhancement alone.

As pointed out by the contributors to this symposium, there are a number of basic problems in atomic and molecular physics that still await solutions. Many of them have surfaced through the long history of the field, but had to be laid to rest quickly because of our lack of suitable (intense and tunable) probes. Now, however, we are standing at the threshold of tackling these problems. One of them is the three-body continuum problem, exemplified by the double photoionization process in helium and the ionization-Auger correlation at inner-shell thresholds. Experimental examination of this phenomenon needs to be carried out at a differentiated level in which the resulting particles are analyzed in energy, direction, and especially in an angular-correlation frame. At the same time, the measurements must approach the threshold where the cross section vanishes. We are at present lacking one to two orders of magnitude in available flux to undertake these experiments.

Autoionizing states, multiple-excitation states, scattering states and shape resonances are often located in the vicinity of thresholds, both inner and outer shell. The study of these states, which generally requires both high resolution and great sensitivity, relates very directly to the problems of multi-channel or multi-configuration interactions. The need for improved conditions is illustrated in Fig. 5-1 for the Rydberg excitation series 5d → nl in atomic mercury. Here, as in many similar cases, one wants to separate the various decay components, which have low cross sections, and determine the natural width of the lines, which may often be smaller than 0.1 meV.

Another example of a study calling for greatly improved resolution is shown in Fig. 5-2. In this case, the various ionization channels in Kr include Auger processes and two-electron ionization events. The disentanglement of these competing and interfering channels goes far beyond our present measurement capabilities. In molecules the multitude of levels and de-excitation pathways imposes even more critical demands on the experimental capabilities if we are to understand the molecular structure and dynamics at a basic level. Fig. 5-3 presents the variation of the angular-distribution parameter for the decay of an excitation series to the ground-state ion of carbon monoxide. At present, the spectral features are resolution limited.

Even in the simplest cases, the photoionizaton process is determined by five parameters--three matrix elements and two phase shifts. Experimentally, a five-parameter experiment can be conducted that allows the determination of these fundamental quantities. However, this experiment, which has been called "complete," comes at a price, as illustrated in Fig. 5-4, because the simultaneous analysis of energy, angle, and spin-polarization parameters leads to a signal strength 10^3-10^4 times smaller than usual, which must be compensated by an increased primary flux of photons. Furthermore, for the determination of two of the spin parameters, the incident radiation must be circularly polarized.

Another example of study requiring greatly improved tuneability is the near-threshold x-ray fluorescence spectroscopy of molecules. The selective excitation of the Cl-containing molecules with polarized synchrotron radiation in the Cl 1s near-threshold region has revealed a diversity of phenomena, including screening and resonant Raman effects below threshold and fluorescence polarization.

While we have presented a few specific and basic experiments which await advanced SR sources, there are other techniques and studies which will benefit as well. A few examples are: time-resolved spectroscopies, translating often into real-time studies; the detection and study of extremely dilute species; photoinduced chemistry; and delineation of the properties of excited states, atomic ions, radicals or intermediate atomic and molecular species, open-shell atoms, and last but not least, plasmas at detailed levels.

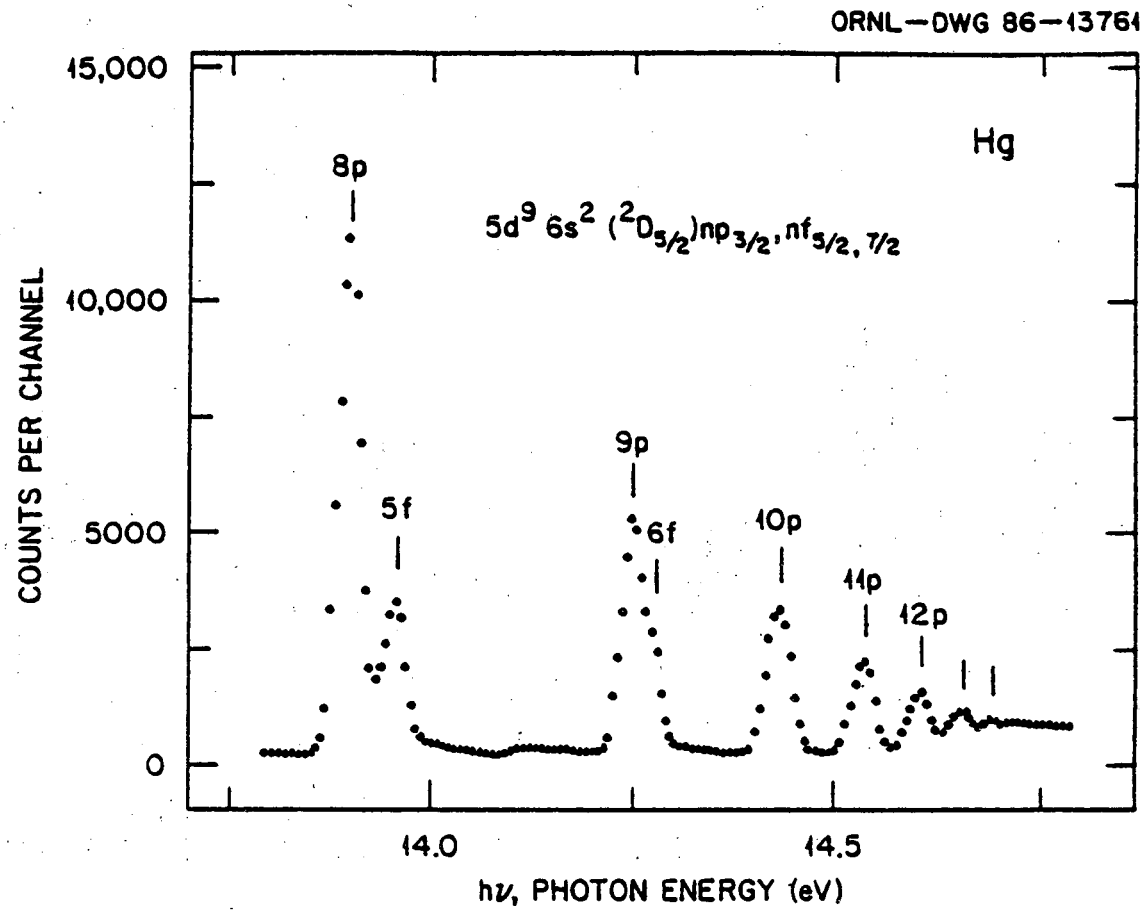


Figure 5-1. Ionization cross section of atomic Hg.

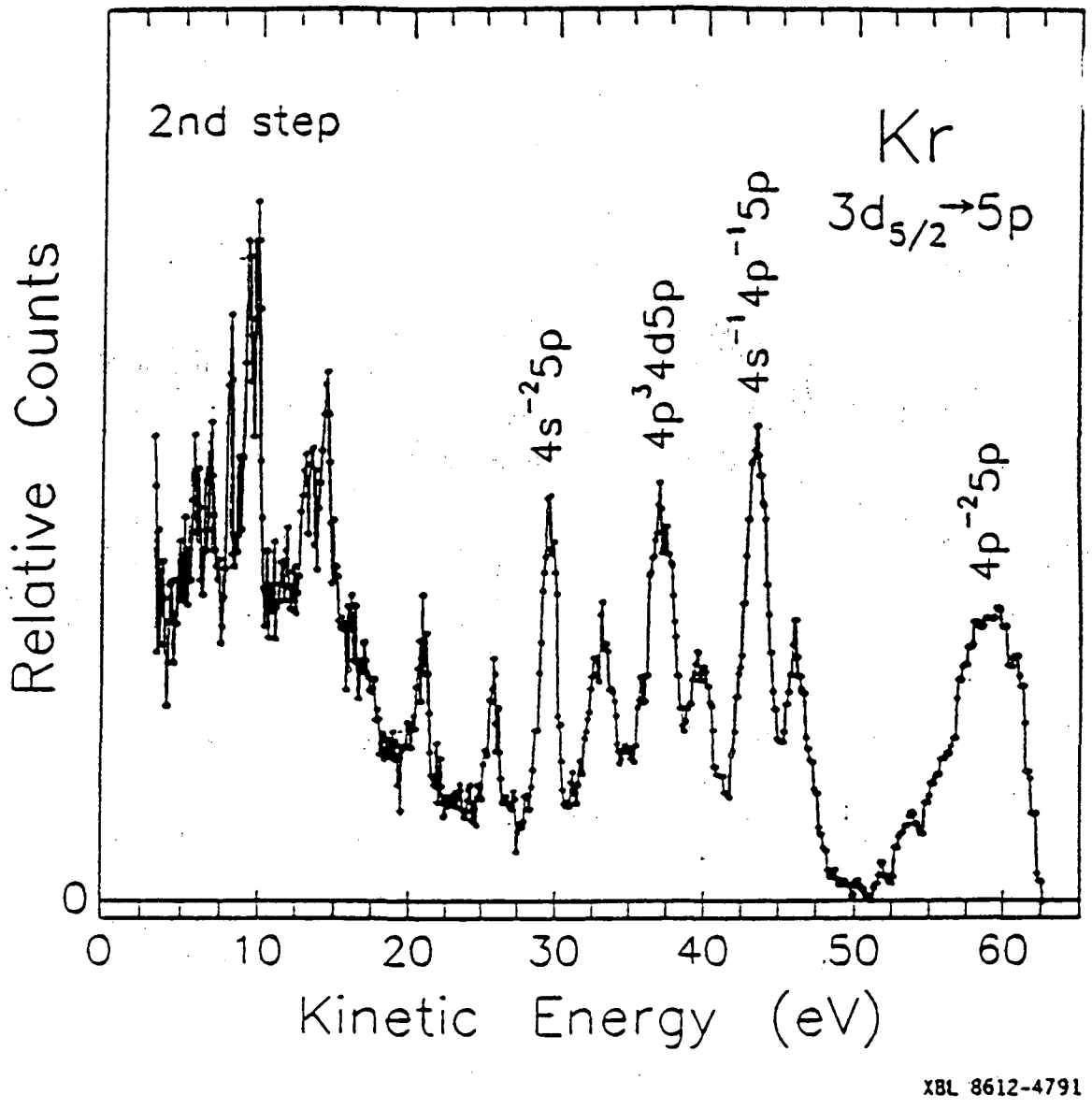


Figure 5-2. Photoelectron spectrum of Kr at the 3d → 5p resonance.

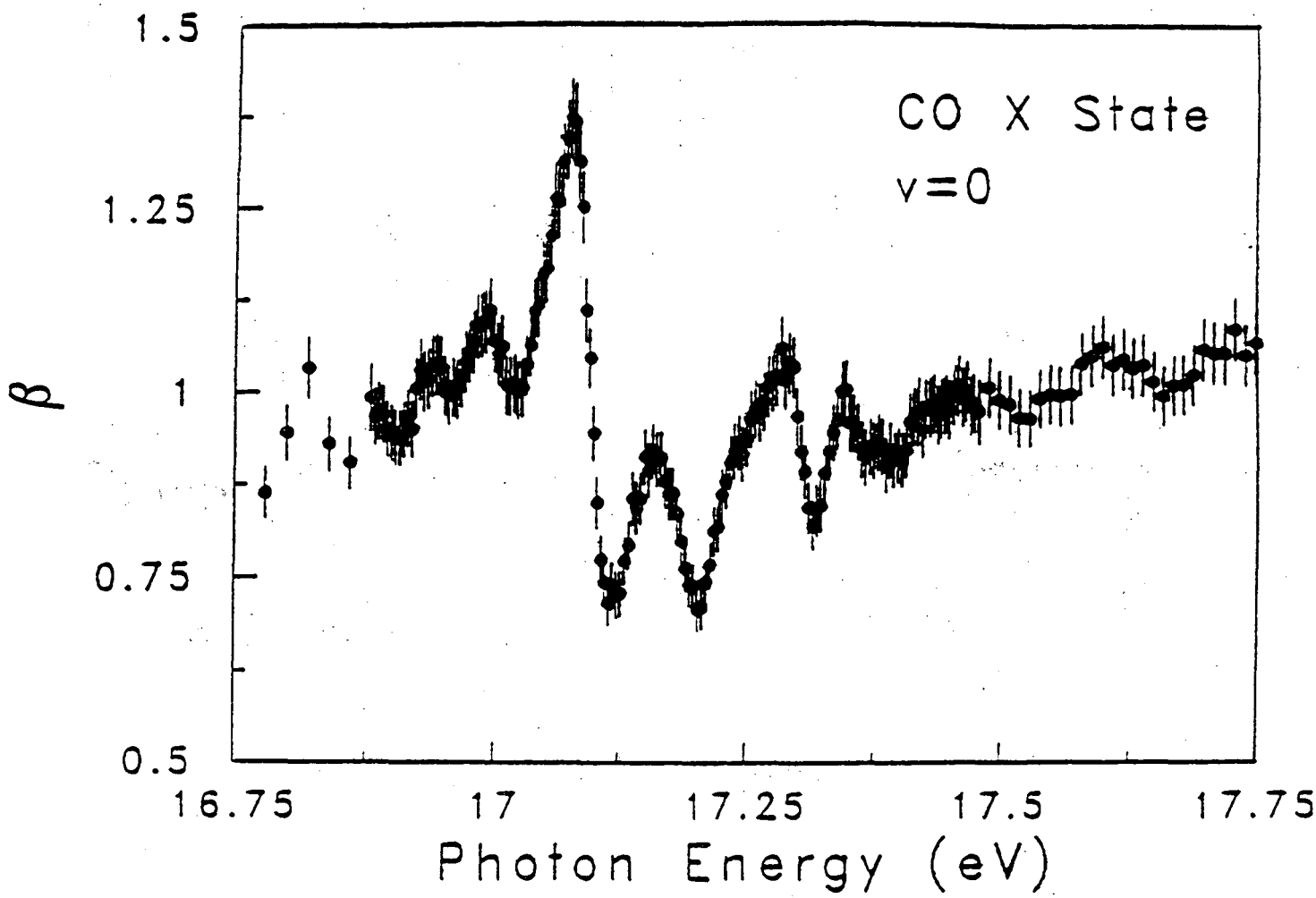


Figure 5-3. Angular distribution parameter of the v = 0 vibrational level of the state of CO.

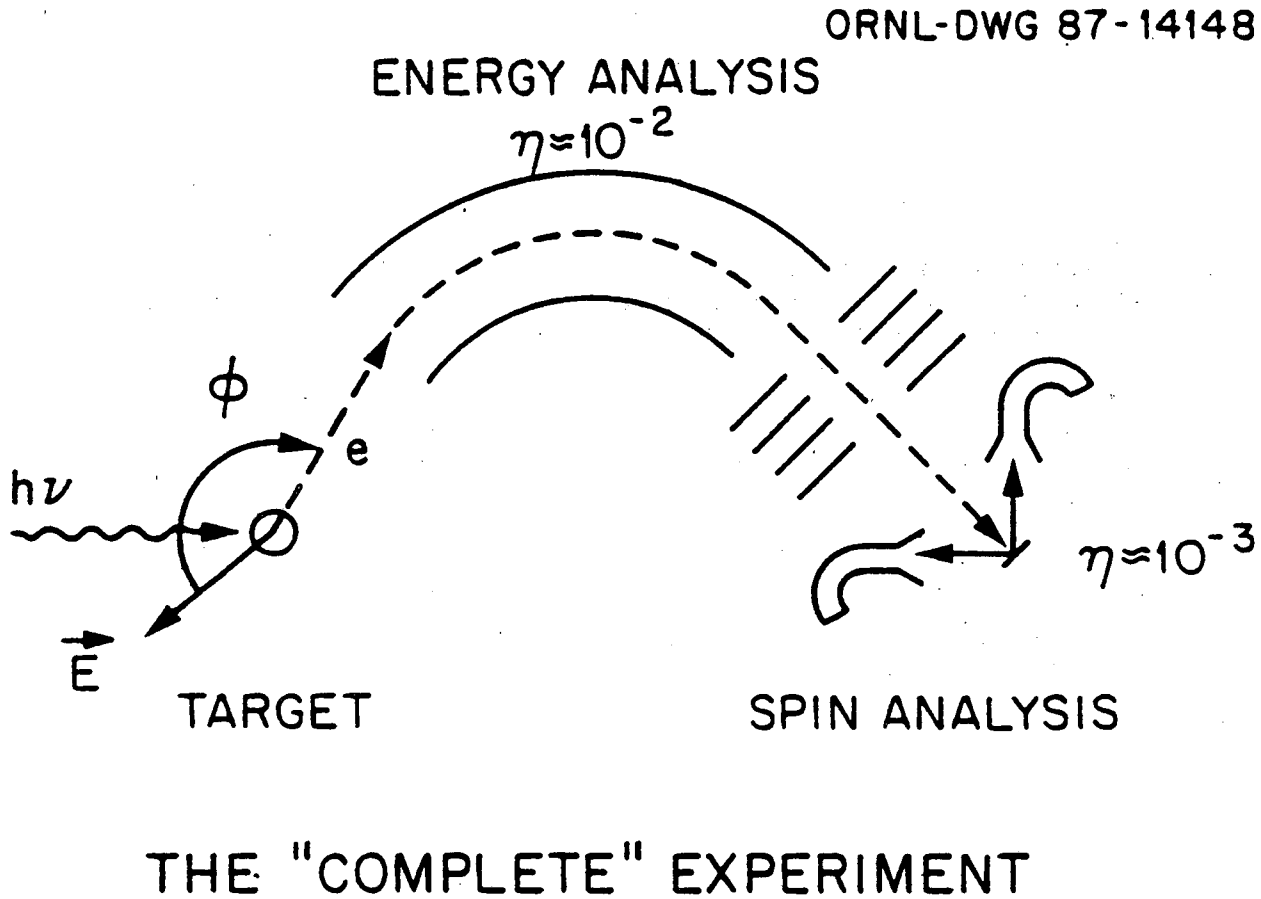


Figure 5-4. Schematic of the "complete" experiment.

The opportunities in the area of research dealt with in this Workshop, and in the field of atomic and molecular science in general, are great and challenging. They warrant special considerations on the part of designers and operators of the photon source. On the other hand, the technical pecularities of the advanced sources impose special considerations on the part of the user. Granted reliable and stable conditions in the photon source (which is a high priority), efficiency becomes a prime factor. This implies excellent preparation of the experiment by the user and rapid switchover times from one user to the next and from one beamline to another. The availability of staging areas is one of the mundane yet practical considerations which deserves special attention at any SR source.

VI. Session 6: Fluorescence

Carl L. Nordling

An overview talk was given at the opening session by R.D. Deslattes on near-threshold phenomena in x-ray fluorescence. With the availability of tunable synchrotron radiation sources, x-ray near-threshold phenomena can now be studied in considerable detail. In addition to realizing the originally formulated goals of the research, a wide array of unexpected phenomena which are specific to the near-threshold and sub-threshold regions have been encountered. Some of these phenomena can be understood rather easily, while others still remain more or less unexplained.

Among the latter category Deslattes mentioned some rather startling changes in the region of the sulfur $K\alpha$ doublet in sulfur hexafluoride which occur when the excitation energy is detuned only slightly from its threshold value. For example, the $K\alpha_1/K\alpha_2$ intensity ratio changes from 2:1 to 1:2 for different excitation energies close to the $1a_{1g}(S\ 1s) \rightarrow 6t_{1u}$ resonance, and a broad line appears which seems to track the photon energy. Also, in chlorine $K\beta$ emission from CF_3Cl, R.C.C. Perera reported drastic and still only partially understood changes in x-ray energies, widths, and relative intensities of the fluorescent peaks when the exciting photon energy is tuned below the ionization threshold into the resonance-excitation region. He tentatively explained the energy shifts and intensity effects in terms of perturbations due to the presence of a spectator electron residing in an unoccupied molecular orbital. The narrow line widths obtained in the spectra excited below threshold were explained in terms of an "effective" hole-production region in a core state limited by the broadening of the unoccupied level. The change in line widths as a function of below-threshold excitation energy was proposed as a novel technique to study the localized properties and reorganization effects of a core hole.

A different way of promoting an electron into a spectator position relative to subsequent x-ray transitions was discussed by P. Springer, who used the process of nuclear electron capture to obtain a spectator valence electron in the daughter atom. The x-rays emitted following the nuclear electron capture are shifted from the daughter's characteristic x-rays by the presence of the spectator electron. The shifts should be largest in the lanthanide and actinide elements where the valence orbitals 4f and 5f lie inside the atom and provide considerable screening for outer-to-inner shell x-ray transitions. Springer and co-workers have observed a shift in the $5p \rightarrow 3s$ transition of dysprosium by comparing the spectrum of x-rays emitted following electron capture in ^{163}Ho with those excited by electron bombardment of dysprosium. The observed shift in the $5p \rightarrow 3s$ transition is -19 eV which is comparable to the frozen-orbital prediction of -25 eV, but not to the relaxed orbital prediction of -5.3 eV.

One new perspective for near-threshold work which is now being realized is the polarization of molecular x-ray fluorescence. Polarization phenomena provide a new means of determining the relative orientations of molecular orbitals, and therefore indicate one of the new directions in soft x-ray

near-threshold phenomena, or as Deslattes phrased it: "We have been seeing the nose of the camel, and the camel's name is polarization." (Fig. 6-1) By tuning the incident x-rays to sub-threshold absorption resonances, using a curved-crystal monochromator with a position sensitive detector, P. Cowan and co-workers were able to populate selected unoccupied molecular orbitals. However, excitation can only occur when the unoccupied orbitals in question are properly oriented with respect to the polarization E-vector of the incident x-rays. In a gas-phase sample, therefore, x-ray absorption will only occur for molecules with appropriate orientation. These excited, oriented gas molecules can subsequently decay by emitting fluorescent x-rays. In most cases this fluorescence occurs very quickly compared to the re-orientation times for the molecules. The polarization of the fluorescence will therefore depend on both the relative orientation of the initially unoccupied orbital and the final-state hole orbital (Fig. 6-2).

J.A.R. Samson reported fluorescence work in argon. Undispersed radiation from the Synchrotron Radiation Center in Wisconsin was used to stimulate 3p → 3s fluorescence. The fluorescent radiation was dispersed by the use of a Seya-Namioka monochromator with a 5 Å bandpass. The relative intensities of the spectra shown in Fig. 6-3 were determined as a percentage of the strong emission line observed at 919.8 Å, produced by the transition

$$3s3p^6(2S) \rightarrow 3s^2 3p^5(2p_{3/2}) + h\nu.$$

The intensities of some of the fluorescent lines are, of course, modified by cascading effects. The lines observed at 767.26 Å and 640 Å do not correlate with any known energy levels of Ar. They have been tentatively assigned to transitions of the type

$$(3s3p^5)nl \rightarrow 3s3p^6 + h\nu.$$

D. Judge addressed the question of where the energy goes in the absorption process, from onset into the x-ray region. In the wavelength region of a few hundred angstroms or less, two-electron transitions (or more than two) are well known. Such two-electron transitions have been investigated in CO using ESCA as well as synchrotron radiation. The identification of these states has been suggested by both Langhoff and Schirmer, although with some differences. Since the resulting ion states are different, any discrepencies could possibly be resolved by observing the radiative decay of the excited ion, if, in fact, radiative decay occurs. Another example of many-electron excitations may be seen in the work of Brion on CO2. Since the emission from such states will generally be weak, high incident photon flux will be required to investigate the importance of competitive processes in the decay of multiple-electron excitations via fluorescence processes.

Less difficult to determine, in CO, but no less important, are the states of the ion species which are formed in the absorption process. At wavelengths shorter than 500 Å, it is possible to form dissociation products which are both ionized and excited. The magnitude of the absolute cross sections for these processes is relatively low, but readily measurable. Such information on the various product channels provides constraints on theoretical models for the physics of the "half-collision" (Figure 6-4).

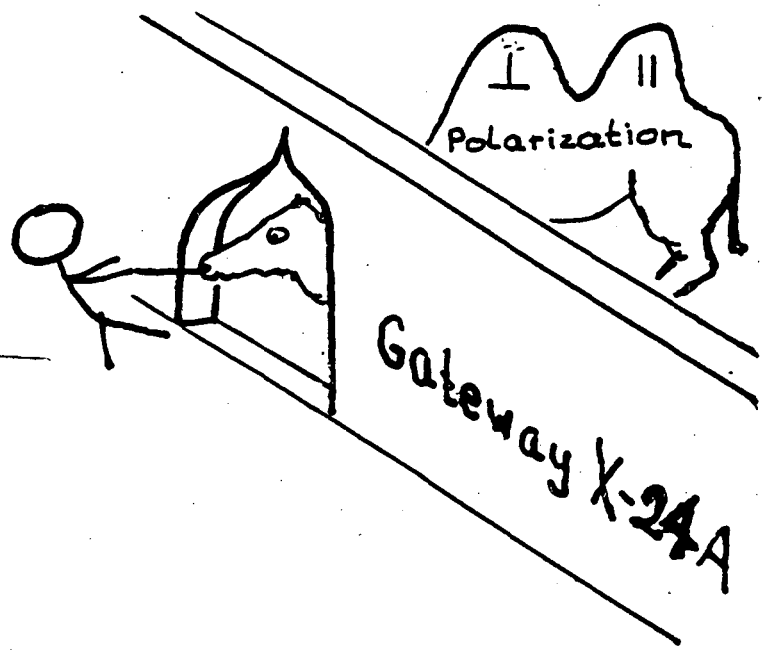
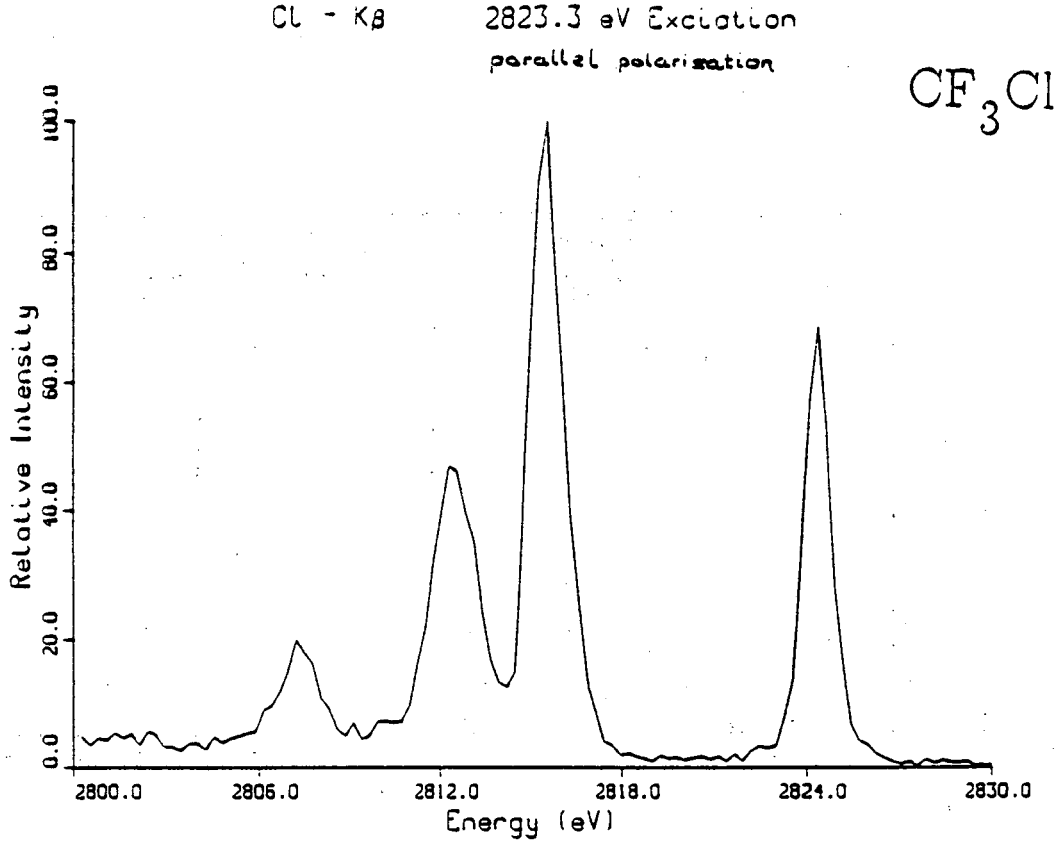


Figure 6-1. "We are seeing the nose of the camel; and the camel's nose is Polarization." (Quotation from "Godfather" Deslattes.)



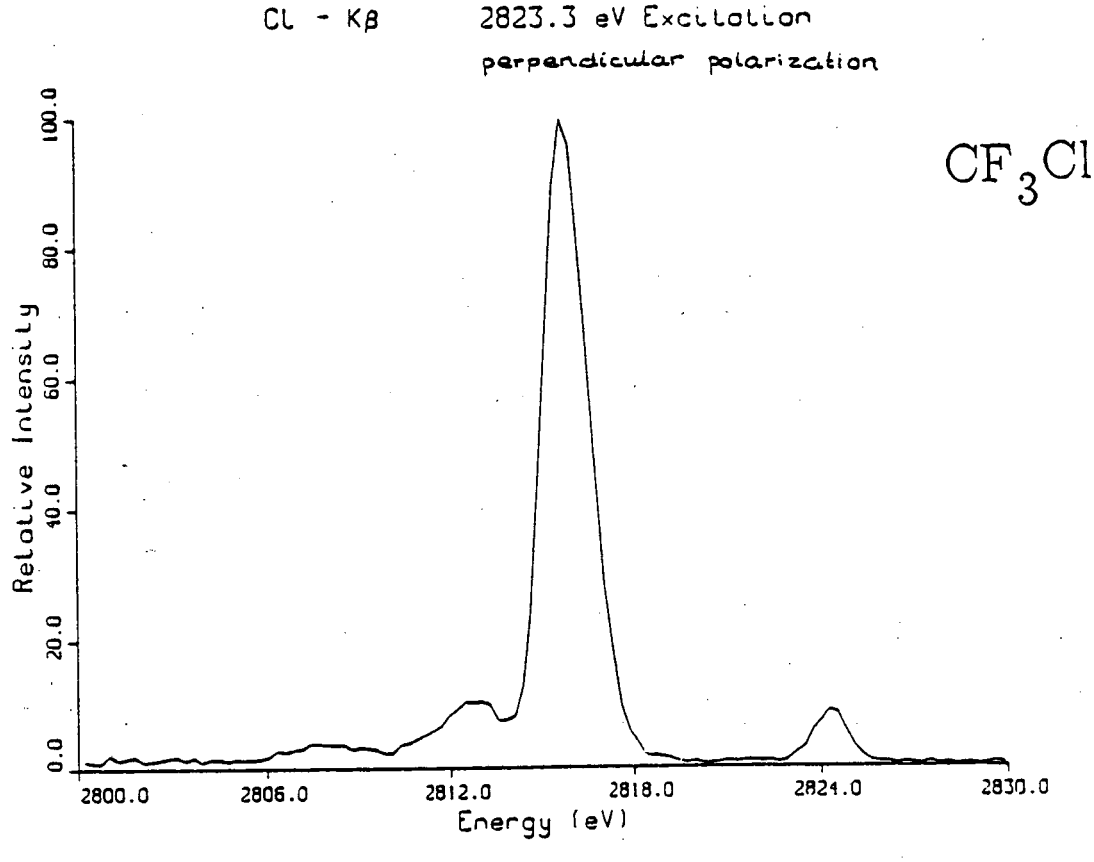
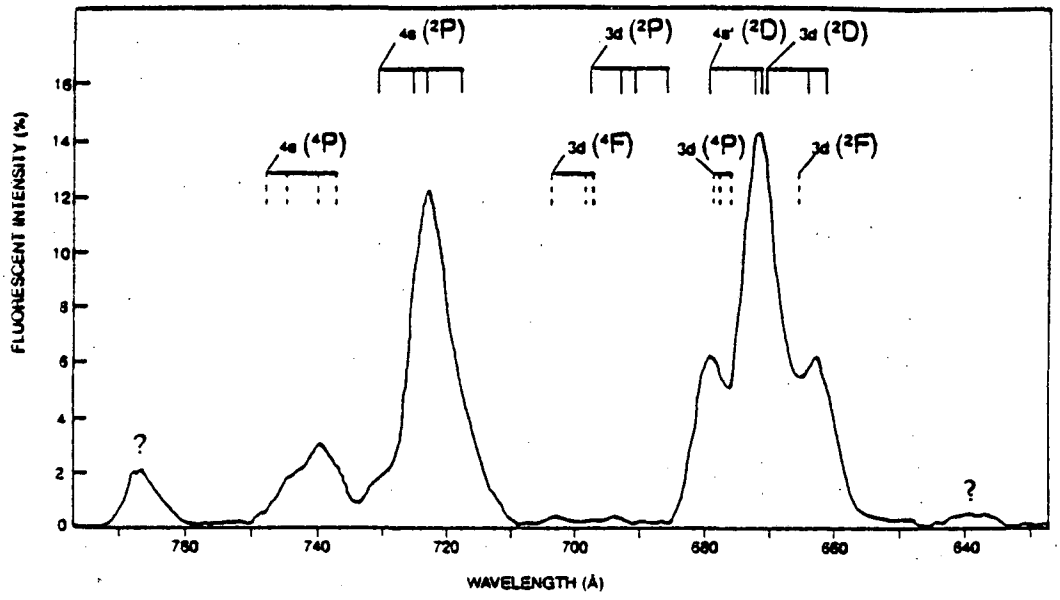


Figure 6-2. Near-threshold polarization effects in CF3Cl. "Parallel" and "perpendicular" refer to polarization of flourescent radiation with respect to polarization of synchrotron radiation.



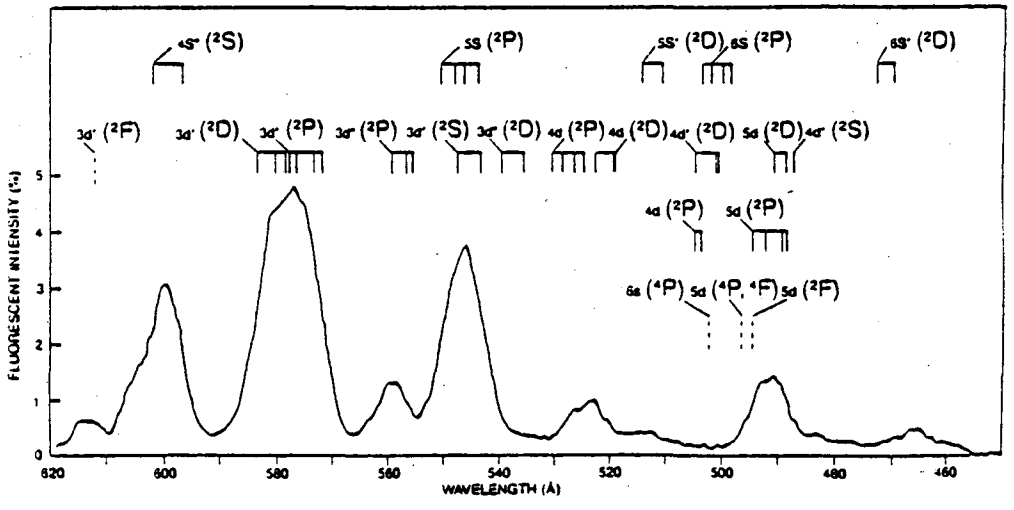


Figure 6-3. Flourescence spectrum emitted from argon satellite states.

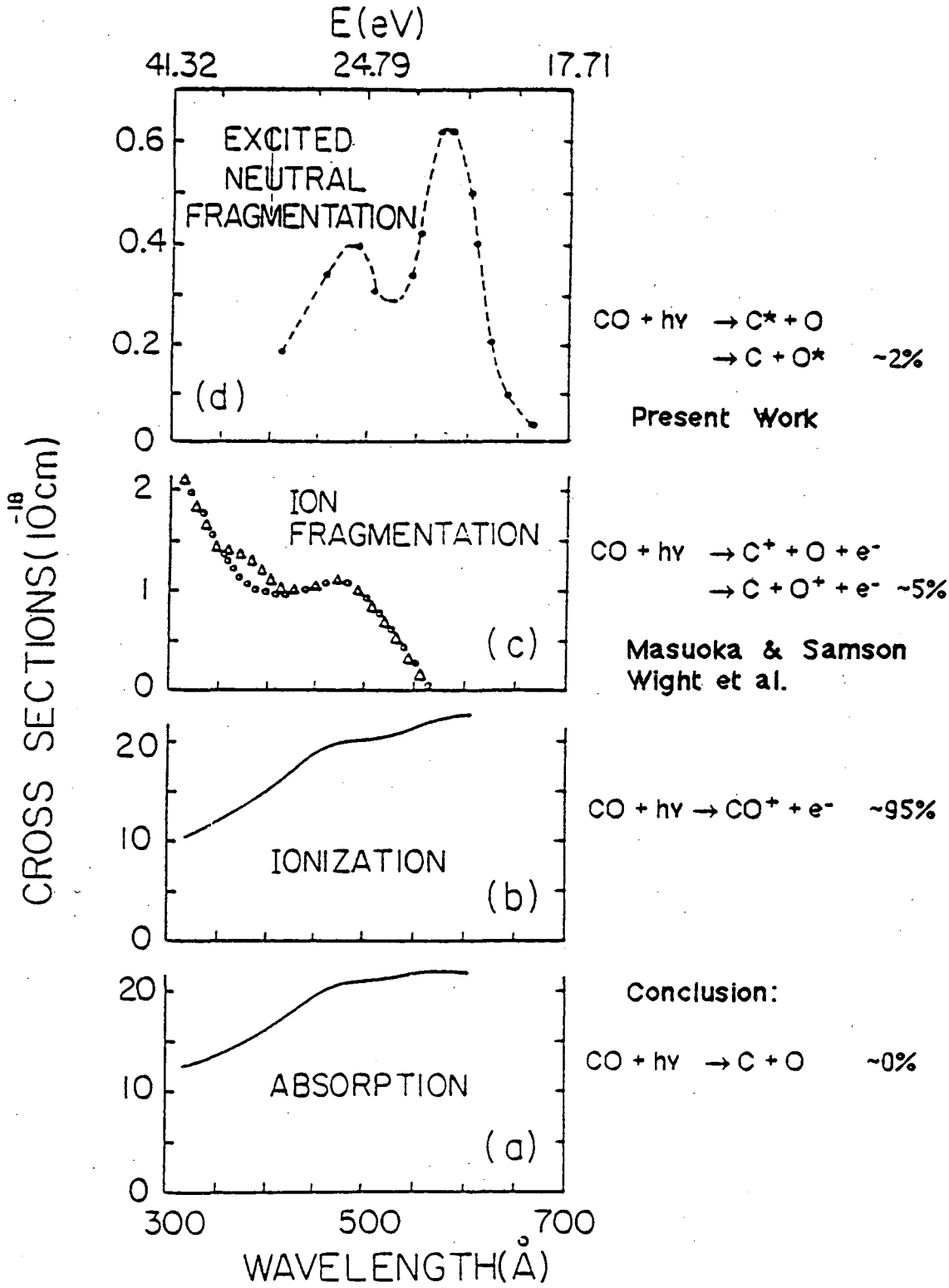


Figure 6-4. CO molecule. Competition between excited neutral fragments and ground state ion fragments in the double-electron excitation region.

A new fluorescence spectrometer with a sensitivity 10^3-10^4 times greater than conventional instruments has been used at the NBS-SURF and NSLS synchrotron-radiation sources to study the partial density of states in a number of materials (Fig. 6-5). D. Ederer reported work on lithium fluoride for which fluorescence was observed from K-V transitions in lithium (Fig. 6-6). Fluorescence from the exciton (1s-2p) at 62 eV also was observed. Synchrotron radiation from SURF with energies greater than 100 eV was used to create the core holes and excitons, making it possible to study their fluorescence as a function of excitation energy.

The high sensitivity of the spectrometer enabled a study of a dilute (~ 1%) alloy mixture of aluminum in magnesium. It was also possible to look at the double-vacancy satellite in magnesium and compare its structure with the aluminum impurity and the KLV Auger spectral shape. According to the equivalent-core approximation the spectral shape of these features should be the same. The experimental results show only qualitative agreement.

J. Nordgren in his talk stresssed the long held hope of combining high-resolution spectroscopy of secondary photons (and electrons) with tunability of the incident radiation, i.e. with selective excitation. In his case the energy range of interest is below 1 keV where fluorescence yields and instrumental efficiencies generally are low. One therefore needs a very high photon flux from the light source and an efficient design of the analyzing apparatus.

Nordgren described a new grazing-incidence instrument covering the wavelength range 10-250 Å (50-1000 eV) (Fig. 6-7). The instrument has been designed according to a new concept which allows a large spectral range to be covered, while still providing high resolution and luminosity. In addition, the instrument offers a high degree of versatility and can be easily adapted to different sources. [J. Nordgren and R. Nyholm, Nucl. Instrum. Meth. A246, 242 (1986)]

The sensitivity of the spectrometer depends on the wavelength and resolution selected, but as a typical example the high-resolution (0.07 eV at 280 eV) sensitivity is 10^{-8}. In low-resolution mode (0.6 eV at 280 eV) the sensitivity is 4×10^{-7}. Since typical yields for soft x-ray fluorescence are in the order of 10^{-4}, an incident flux of 10^{11} to 10^{13} sec^{-1} is required on the sample. This can be achieved in a fine focusing electron beam and even in a beam of monochromatized photons from a wiggler or undulator at a storage ring. First experiments have been completed recently at the Flipper monochromator at the HASYLAB multipole wiggler. For example, threshold-excited Cu L and O K emission spectra of high-Tc superconductors were recorded. Also, resonant behavior in Ti L fluorescence has been observed.

Nordgren also discussed a case where dynamic molecular effects could be studied by choosing an appropriate molecular system. In the carbon K emission from CO the phase of the wave function of the intermediate state, i.e. the initial state of the x-ray transition, becomes important. Due to interference between the different excitation channels the vibrationally resolved x-ray spectrum becomes modified. This rather subtle effect can be examined when high-resolution spectra become available. Finally, Nordgren suggested that it may be possible with his new instrument to do Bremsstrahlung Isochromat Spectroscopy (BIS), (or Inverse Photoemission), in particular to study resonant BIS (i.e. $E_{kin} \simeq E_{core}$) in the energy region 100 eV - 1 keV. Most previous BIS work has been done either below 50 eV or at 1487 eV, where interfering core excitations are absent.

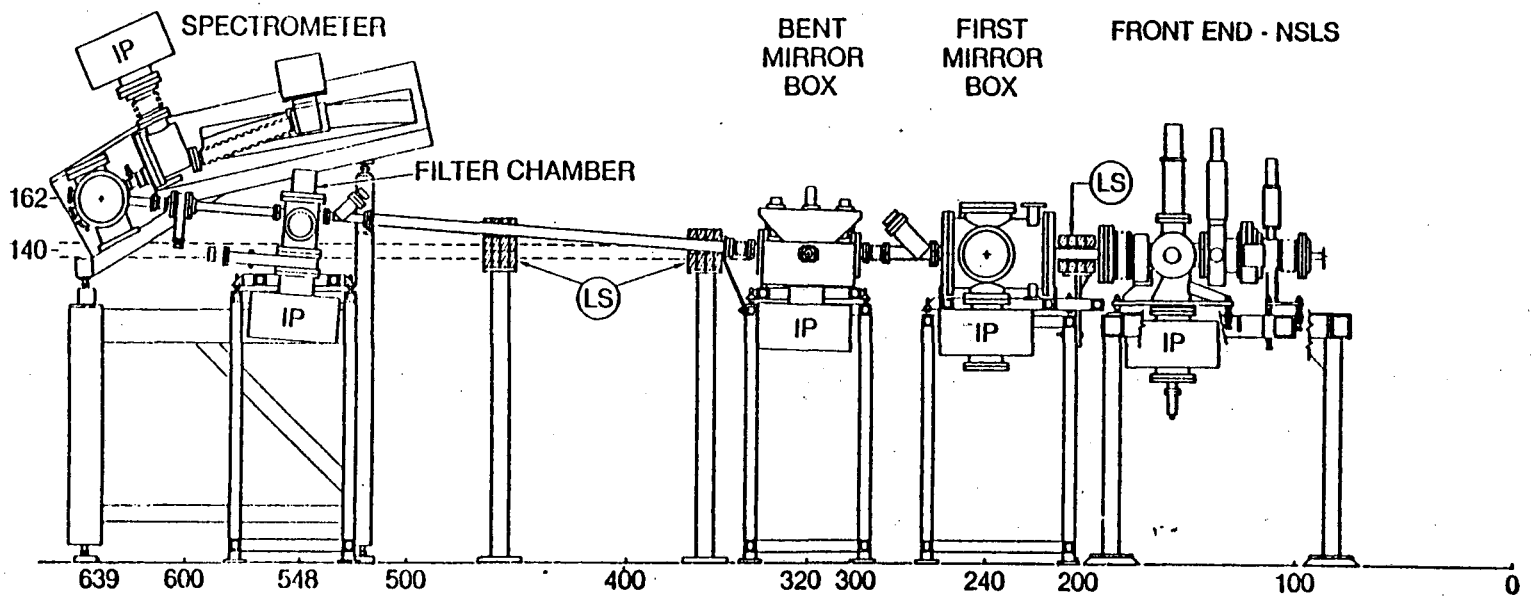


Figure 6-5. Diagram of synchrotron radiation light beamline used for photon excitation with soft x-rays (energies below 1000 eV).

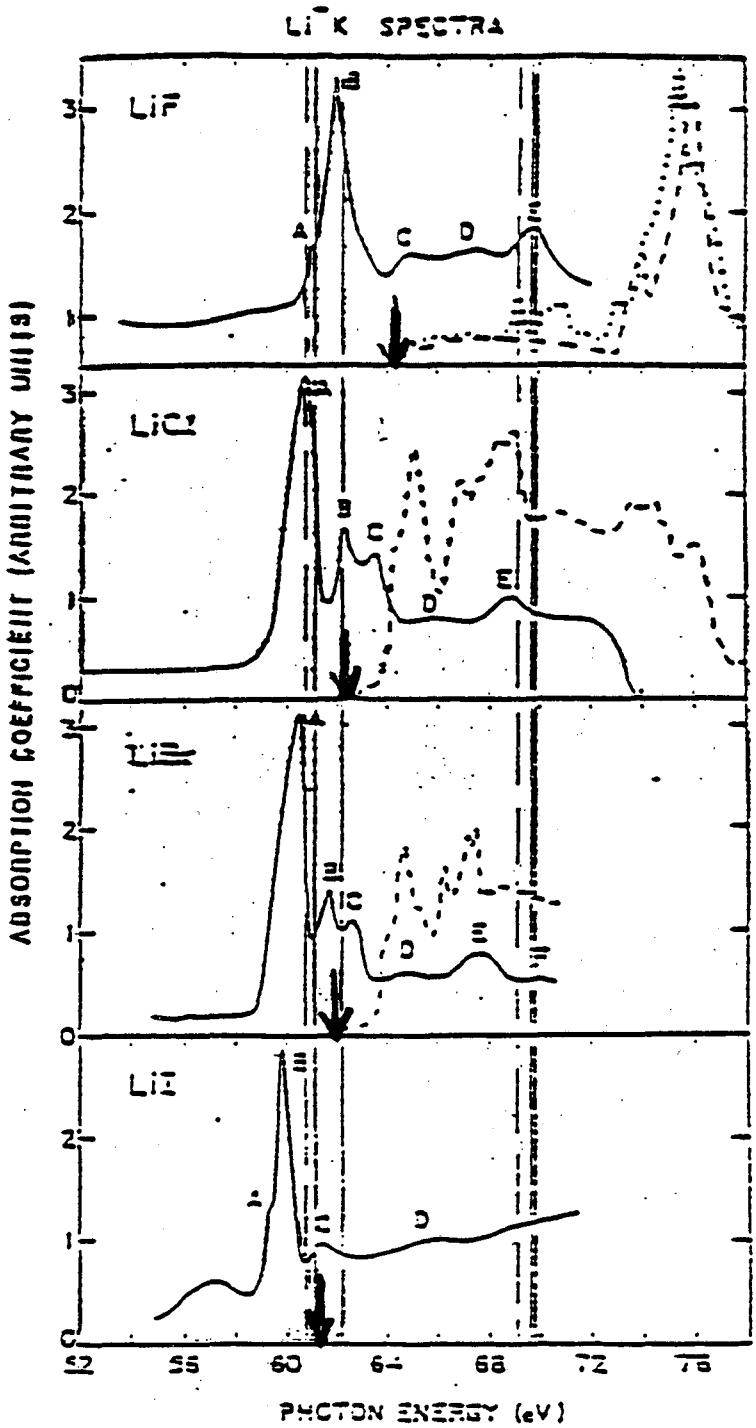


Figure 6-6. XUV exciton flourescence from LiF.

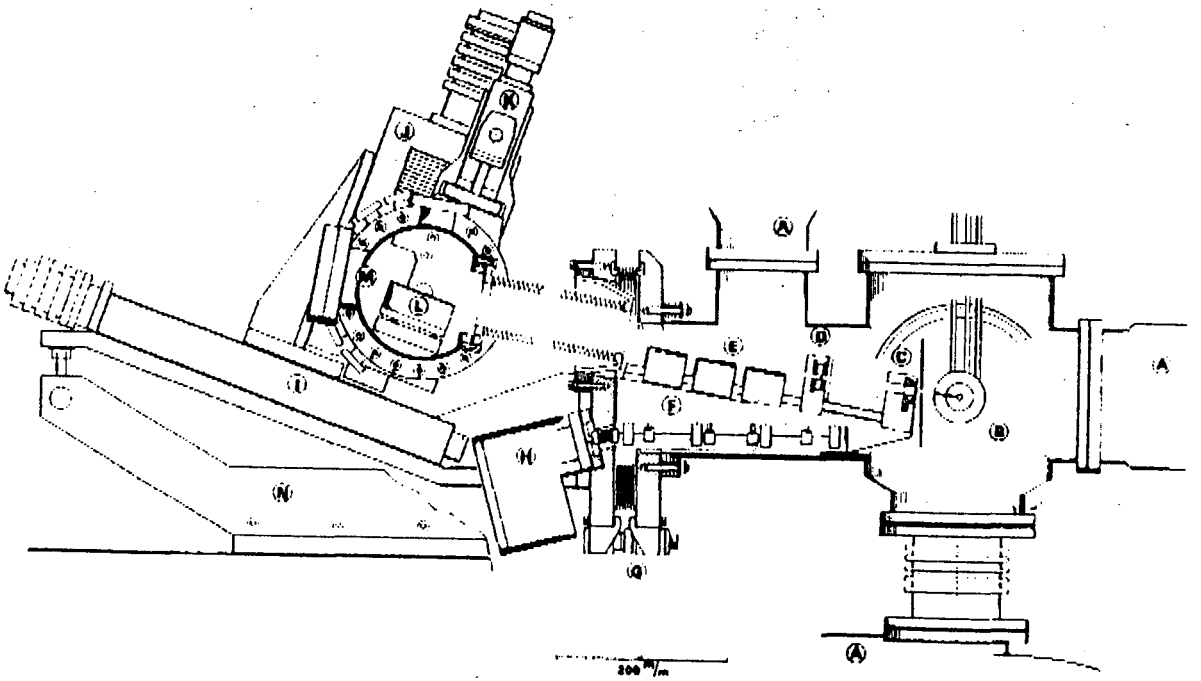


Figure 6-7. Outline of the multi-grating grazing-incidence instrument. A: Vacuum pumps B: Sample Holder, C: Entrance slit, D: Grating Selector, E: Gratings, F: Reference Block, G: Optical axis adjustment, H: Rotational feedthroughs, I,J,K: Translational stages, L: Detector, M: Detector housing, N: Support structure.

VII. Session 7a: Anomalous Scattering

Richard L. Blake

Although only three papers were included in this session the topics covered a wide range of applications of x-ray scattering, both normal and anomalous. There were papers by B.L. Henke, J.B. Kortright, and J. Kirz.

The atomic scattering factor is written in terms of real and imaginary parts as

$$f = f_0 + f' + if'',$$

where f_0 is referred to as the normal part that has angular dependence. A consensus seemed to emerge from the 1985 Asilomar meeting that f′ and f″ were independent of angle within bounds of a few percent at low to intermediate energies, but could have as much as ten percent angle-dependent contribution at 60 keV (as shown by Shumacher). In order to provide compact tabulations as a function of energy alone, Henke writes the atomic scattering as

$$f = f_1 - \delta f_0 + if_2$$

for low energies, where $f_1 = f' + Z$, $\delta f_0 = Z - f_0$, and $\delta f_0 \rightarrow 0$ for sufficiently low energies. He then tabulates f_1 and f_2 over the low-energy range.

Henke formulates several important radiation-matter interactions in terms of the real and imaginary parts f_1 and f_2, including:

(1) The scattering of x-rays from small particles,

(2) Amplitudes reflected and transmitted by a layer of atoms,

(3) Reflected and transmitted amplitudes for N layers of unit cells, including all multiple reflections,

(4) Dynamical diffracted transmission and reflection intensities,

(5) Transmitted and reflected intensities from mirrors, molecular multilayers, and periodic multi-layered structures,

(6) Photoemission yields of photocathodes, and

(7) Responses of photographic films.

For the various applications of atomic scattering factors Henke has always maintained an absolute calibration program to verify the models he developed for each application. Applications outside the range 100-2000 eV require additional tabulations such as Cromer and Liberman that include angular dependence.

Kortright has helped develop a new application of x-ray scattering to structural studies of binary amorphous alloys. He has measured the angular distribution of synchrotron radiation scattered from Mo-Ge films. By using two (or preferably more) energies near the K edges where anomalous scattering is large he is able to solve a set of equations for partial scattering functions. The angular dependence now gives information on the locations of atoms with respect to one another, i.e. structural information. Transformations applied to the data yield radial-distribution functions, hence structural information on atomic positions. He shows that the anomalous-scattering technique can provide accurate quantitative results that are complementary to EXAFS results. Anomalous scattering covers a range of wave-vector (k) space near the origin while EXAFS is sensitive to the high-k region.

Janos Kirz emphasized that dominant features in atomic scattering factors carry over into the optical constants of materials and can be used for improved x-ray optical systems. Three significant applications were reviewed.

(1) By match of materials and region of interest it is possible to achieve a material such that phase zoneplates and diffraction gratings have optimized efficiency,

(2) Diffraction patterns on non-periodic materials, such as a single biological cell, may be interpretable for image reconstruction. An example was shown where the processed diffraction pattern from a muscle cross section contained rings corresponding to a spacing of about 60 nm, and

(3) Peaks in k can be used to improve contrast in x-ray microscopy. A nice example used the white-line structure at the Ca $L_{II,III}$ absorption-edge to provide high contrast for mapping Ca in bone via scanning microscopy.

Appendix I

WORKSHOP ON NEW DIRECTIONS IN SOFT X-RAY NEAR THRESHOLD PHENOMENA

March 1-4, 1987

Final Agenda

Sunday, March 1

1630 Reception

1800 Dinner

1930 Session 1: Opening

Organized and Chaired by: Richard Pratt

Michael Moran (LLNL)
Welcome

Richard D. Deslattes (NBS)
"X-ray Fluorescence Near Threshold" (40 mins.)

Teijo Aberg (Helsinki)
"Origin of X-Ray Fluorescence and Auger Electron Emission" (40 mins.)

David A. Shirley (LBL)
"Gas-Phase Photoemission: Some New Directions in Electron-Correlation Phenomena" (40 mins.)

Monday, March 2

0730 Breakfast

0830 Session 2a: Photoabsorption

Organized by: Nancy Kerr Del Grande
Chaired by: Glenn Tirsell

Chris E. Brion (U. British Columbia)
"Absolute Cross Sections for Molecular Photoabsorption, Partial Photoionization, and Ionic Photofragmentation Processes: A Comparison of Photon and Dipole Electron-Impact Methods" (20 mins.)

Christiane Bonnelle (Paris)
"Photoabsorption and Anomalous Scattering of X-Ray Resonant States" (20 mins.)

Nancy Kerr Del Grande (LLNL)
"Near-Threshold Photoabsorption: Resonances, 'White Lines', and Other Enhancements" (10 mins.)

Sesson 2b: Photoionization I

Organized by: Bernd Crasemann
Chaired by: John West

Teijo Åberg (Helsinki)
"Theory of PCI" (25 mins.)

Volcker Schmidt (Freiburg)
"Current Directions in PCI Phenomena" (25 mins.)

1200 Lunch

1700 Wine and cheese

1800 Dinner

1930 Session 3: Photoionization II

Organized by: Thomas A. Carlson
Chaired by: John West

Thomas A. Carlson (ORNL)
"Angle-Resolved Electron Spectroscopy Studies in the Pre-Ionization Region" (30 mins.)

G. Michael Bancroft (U. Western Ontario)
"Gas-Phase Spectroscopy at Si 2p and Ar 2p Core Levels" (10 mins.)

Wolfgang Eberhardt (EXXON)
"Core-Electron Excitation and Decay in Molecules" (20 mins.)

Tricia A. Ferrett (NBS)
"Shake-Up, Shake-Off, and Shape-Resonance Effects in Near-Threshold Photoionization" (30 mins.)

Fred Grimm (U. Tennessee)
"Theory of Molecular Shape Resonances" (20 mins.)

Chris E. Brion (U. British Columbia)
"High-Resolution PES Studies of the Ar 3s Satellite Spectrum" (10 mins.)

Tuesday, March 3

0730 Breakfast

0830 Session 4: Theory

Organized by: Steven T. Manson
Chaired by: Peter W. Langhoff

David Smith (U. Vermont)
"Theoretical and Experimental Studies of the Relationship of Photon Scattering and Photoabsorption" (25 mins.)

Anthony F. Starace (U. Nebraska)
"Theoretical Overview of Near-Threshold Photoionization" (25 mins.)

Göran Wendin (Göteborg)
"Resonance and Threshold Emission Processes in Electron-Impact Excitation of Solids" (25 mins.)

Lynn Kissel (Sandia)
"Atomic Rayleigh Scattering Near Threshold" (25 mins.)

Yoshihiro Ohmura (Tokyo)
"Near-Edge Structure in Gamma-Ray Inelastic Scattering by K-Shell Electrons in Heavy Elements" (25 mins.)

1200 Lunch

1430 Session 5: Future Capabilities Offered by Advanced Synchrotron Radiation Sources

Organized by: Manfred O. Krause
Chaired by: Wolfgang Eberhardt

David T. Attwood (LBL) Opening

Ernst E. Koch (BESSY)
"New Opportunities in Chemical Spectroscopy with Advanced Synchrotron Radiation Sources (20 mins.)

Albert C. Parr (NBS)
"New Opportunities for Angle-Resolved Photoelectron Spectroscopy of Molecules Afforded by Newly Planned Light Sources" (20 mins.)

Steven T. Manson (Georgia State U.) and Dennis W. Lindle (NBS)
"Atomic Physics with an Intense Synchrotron Radiation Source: Theoretical and Experimental Aspects of the Emerging Possibilities" (25 mins.)

1700 Wine and cheese

1800 Dinner

1930 Session 6: Fluorescence Spectroscopy

Organized by: James A.R. Samson
Chaired by: Richard D. Deslattes

Joseph Nordgren (Uppsala)
"Threshold Soft X-Ray Spectroscopy" (20 mins.)

Paul Cowan (NBS)
"Polarization of Molecular X-Ray Fluorescence" (20 mins.)

David L. Ederer (NBS)
"Soft X-Ray Fluorescence from Low-Z Materials" (20 mins.)

Paul Springer (LLNL)
"Enhanced Interaction Energy Shifts in the X-Ray Spectrum of $_{163}$Ho" (20 mins.)

Darrell Judge (USC)
"Molecular Multichannel Excitation Processes in the XUV" (10 mins.)

James A.R. Samson (U. Nebraska)
"Fluorescence Studies of Satellite States" (20 mins.)

Rupert C.C. Perera (LBL)
"X-Ray Emission Spectra from Highly Excited Neutral Molecules: Screening Effects" (10 mins.)

Wednesday, March 4

0730 Breakfast

0830 Session 7a: Anomalous Scattering

Organized by: Jeffrey B. Kortright
Chaired by: David Smith

Burton L. Henke (LBL)
"A Semi-Empirical Description of Low-Energy X-Ray Interactions with Condensed Matter: Photoabsorption, Scattering, Specular and Bragg Reflections" (25 mins.)

Jeffrey B. Kortright (LBL)
"Binary Amorphous Alloys Studied with Anomalous Scattering" (20 mins.)

Janos Kirz (Stony Brook)
"What Anomalous Dispersion and X-Ray Dispersion can do for Soft-X-Ray Imaging" (10 mins.)

Session 7b: Closing

Organized by: Richard Pratt
Chaired by: Marvin Weber

Session Reviews (5-10 mins. each):

2a.	Ingolf Lindau (Stanford U./SSRL)
2b. & 3.	Peter Langhoff (Indiana U.)
4.	Richard Pratt (U. Pittsburgh)
5.	Manfred O. Krause (ORNL)
6.	Carl Nordling (Uppsala)
7a.	Richard Blake (LANL)

Closing

1200 Lunch

Appendix II

Workshop on New Directions in Soft X-Ray Near-Threshold Phenomena

Program Committee

R.H. Pratt (Chair)	University of Pittsburgh
D.T. Attwood	Lawrence Berkeley Laboratory
R.L. Blake	Los Alamos National Laboratory
C.E. Brion	University of British Colombia
T.A. Carlson	Oak Ridge National Laboratory
N. Kerr Del Grande	Lawrence Livermore National Laboratory
M. Gavrila	FOM Institute, Amsterdam, The Netherlands
B.L. Henke	Lawrence Berkeley Laboratory
E.E. Koch	BESSY, Berlin, West Germany
M.O. Krause	Oak Ridge National Laboratory
I. Lindau	Stanford Synchrotron Radiation Laboratory
S.T. Manson	Georgia State University
C. Nordling	University of Uppsala, Sweden
J.A.R. Samson	University of Nebraska
J.H. Scofield	Lawrence Livermore National Laboratory
D.A. Shirley	Lawrence Berkeley Laboratory

Organizing Committee

D.W. Lindle (co-chair)	Lawrence Berkeley Laboratory
R.C.C. Perera (co-chair)	Lawerence Berkeley Laboratory
C.H. Poppe	Lawrence Livermore National Laboratory
W.J. Shotts	Lawrence Livermore National Laboratory

Appendix III

Teijo E.W. Aberg
Laboratory of Physics
Helsinki University of Technology
02150 ESPOO
Helsinki, Finland

David Attwood
Lawrence Berkeley Laboratory
1 Cyclotron Road
Berkeley, CA 94720

G. Michael Bancroft
Department of Chemistry
Univ. of Western Ontario
London, ON, Canada N6A 5B7

Jochen Barth
Visiting at:
BESSY
Lentzeallee 100
D-1000 Berlin 33
West Germany

Richard L. Blake
Los Alamos National Lab
P. O. Box 1663
Los Alamos, NM 87545

Christiane Bonnelle
Universite Pierre et Marie Curie
Laboratoire de Chimie Physique
11, Rue Pierre et Marie Curie
75231 Paris Cedex 05
France

Chris E. Brion
Dept. of Chemistry
University of British Columbia
2036 Main Mall
Vancouver, British Columbia V6T1Y6
Canada

Thomas A. Carlson
Oak Ridge National Lab
P. O. Box X
Oak Ridge, TN 37831

Mau Hsiung Chen
Lawrence Livermore National Lab
Livermore, CA 94550

Kwok-Tsang Cheng
Lawrence Livermore National Lab
Livermore, CA 94550

John W. Cooper
Natl. Bureau of Standards,
Gaithersburg
Gaithersburg, MD 20899

Paul L. Cowan
Natl. Bureau of Standards,
Gaithersburg
Gaithersburg, MD 20899

Nancy Kerr DelGrande
Lawrence Livermore National Lab
Livermore, CA 94550

Richard Deslattes
Natl. Bureau of Standards,
Gaithersburg
Gaithersburg, MD 20899

Wolfgang Eberhardt
Exxon Research & Engineering Co.
Rte 22 East
Annadale, NJ 08801

David L. Ederer
Natl. Bureau of Standards,
Gaithersburg
Gaithersburg, MD 20899

Tricia Anne Ferrett
Physics Department
Natl. Bureau of Standards,
Gaithersburg
Gaithersburg, MD 20899

Fred A. Grimm
Dept. of Chemistry
University of Tennessee
Knoxville, TN 37996

Burton L. Henke
AFRD
Lawrence Berkeley Laboratory
1 Cyclotron Road
Berkeley, CA 94720

Yoshihiro Ohmura
Tokyo Institute of Technology
Oh-Okayama 2-12-1, Meguro-ku
Tokyo 152, Japan

Albert C. Parr
Natl. Bureau of Standards,
Gaithersburg
Gaithersburg, MD 20899

Rupert C. Perera
Lawrence Berkeley Laboratory
1 Cyclotron Road
Berkeley, CA 94720

Richard H. Pratt
Dept. of Physics & Astronomy
University of Pittsburgh
Pittsburgh, PA 15260

Balazs F. Rozsnyai
Lawrence Livermore National Lab
Livermore, CA 94550

James A.R. Samson
Dept. of Physics & Astronomy
University of Nebraska
Lincoln, NE 68588

Volcker Schmidt
Universitaet Freiburg
Fakultaet Fuer Physik
Hermann-Herder-Strasse 3
7800 Freiburg, Germany

M. Schneider
Lawrence Livermore National Lab
Livermore, CA 94550

James H. Scofield
Lawrence Livermore National Lab
Livermore, CA 94550

David A. Shirley
Lawrence Berkeley Laboratory
1 Cyclotron Road
Berkeley, CA 94720

David Young Smith
Univ. of Vermont
Dept. of Physics
Burlington, VT 05405

Paul Springer
Lawrence Livermore National Lab
Livermore, CA 94550

Anthony F. Starace
Dept. of Physics & Astronomy
University of Nebraska
Lincoln, NE 68588

Agneta W. Svensson
Daresbury Nuclear Physics Lab
Daresbury, Warrington
Cheshire WA4 4AD, England

K. Glenn Tirsell
Lawrence Livermore National Lab
Livermore, CA 94550

Walter J. Trela
Los Alamos National Lab
P. O. Box 1663
Los Alamos, NM 87545

Marvin J. Weber
Lawrence Livermore National Lab
Livermore, CA 94550

Goran Wendin
Chalmers University of Technology
Institute of Theoretical Physics
S-412 96 Goteborg
Sweden

John B. West
Science & Engineering Res. Council
Daresbury Nuclear Physics Lab
Daresbury, Warrington
Cheshire WA4 4AD, England

Joe Wong
Lawrence Livermore National Lab
Livermore, CA 94550

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LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720