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Workshop Report on  
New Directions in X-Ray Scattering\*

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## ABSTRACT

This report is a summary of the Workshop on New Directions in X-Ray Scattering held at the Asilomar Conference Center, Pacific Grove, Calif., April 2-5, 1985. The report primarily consists of the edited transcript of the final review session of the workshop, in which members of a panel summarized the proceedings. It is clear that we are close to achieving an accurate theory of scattering in independent particle approximation, but for edge regions, there is need to go beyond this approach. Much of what is experimentally interesting in scattering is occurring between the photoabsorption edge and the photoelectric threshold. Applications in condensed matter and biological and chemical material studies are expanding, exploiting higher intensity sources and faster time resolution as in magnetic scattering and surface studies. Storage rings are now conventional sources, and new high-intensity beam lines are under development; the free electron laser is one of the more speculative sources. Recent work in x-ray scattering has led to advances in x-ray optics, and conversely, advances in x-ray optics have benefitted our understanding of x-ray scattering.

## INTRODUCTION

L-Division of the Lawrence Livermore National Laboratory hosted the Workshop on New Directions in X-Ray Scattering at the Asilomar Conference Center in Pacific Grove, Calif., April 2-5, 1985. The workshop was attended by 51 participants representing 27 institutions in 7 countries (see Appendices A and B). This was the second of a series of workshops; the Workshop on New Directions in Soft X-Ray Photoabsorption was conducted at the same location, April 8-11, 1984.

The scattering workshop was held to assess the current status of x-ray scattering studies; identify key technical problems in theory and experiment and the resources needed to solve them; promote communication; and stimulate activity in the field.

In the final sessions, the panel reviewed the main workshop topics. These talks, which were typed, transcribed, and edited, form the main body of this report, which is preceded by an executive summary. The executive summary spotlights a few key issues from each of the sessions.

## EXECUTIVE SUMMARY

We are close to achieving an accurate theory of elastic photon-atom scattering in independent particle approximation, as in the work of Kissel and Liberman. However, with the focus of interest on edge regions, the need to go beyond simple independent particle approximation is increasingly evident. The relativistic time-dependent local density approach of Zangwill, Doolen, and Liberman was discussed at the workshop. Some guidance in the construction of improved theories is provided by the general sum rule constraints discussed by Smith. When one considers scattering in a solid or a plasma, Koelling argued that we are dealing with relatively short-range excitations in a long-range structure, and that we should think of imbedded atoms as in an impurity problem.

Numerous new experimental techniques were mentioned, including segmented monochromators, time-resolved studies, interferometric methods, and polarization studies. There are unresolved problems in the scattering from

real substances, as discussed by Gaines. Templeton emphasized that much of what is interesting in scattering is occurring in between the photoabsorption edge and the photoelectric threshold. He also argued that experimentalists who are determining scattering from absorption measurements should utilize dispersion relations for the differences from some model theory.

Many applications of scattering--in condensed matter physics, biological materials, and chemical materials--are now becoming feasible owing to the rapidly expanding experimental capabilities. A number of examples in the condensed matter area were discussed, including magnetic scattering and surface studies. One can now look at very small subtle scattering effects, giving extremely weak signals, as sources of information on important properties of materials. It will be possible to study materials in lower concentrations and to improve measurements of crystal structures of proteins, exploiting higher intensity sources that require less illumination time and do less damage. Time-resolved experiments also have led to many applications.

Electron storage rings can now be regarded as conventional sources of x rays. New high-intensity beam lines are under development; circularly polarized radiation will be available with the development of x-ray wave length quarter-wave plates. More speculative sources include the free electron laser.

These advances are also leading to advances in x-ray optics. Conversely, it is also the progress in x-ray optics that has made many of these advances possible.

## SESSION 6B: PANEL REVIEW OF SESSIONS

### Session 6B.1

#### SESSION 2. THEORY: CAPABILITIES AND PROSPECTS, REVIEWED

Richard Pratt, University of Pittsburgh

In discussing the prospects of theory, since I'm teaching the history of physics this term, I should give a few historical remarks. But, I'll mainly review the status of theory, as we've heard about it at this conference, in terms first of elastic scattering. First, some general ideas we've heard about, then some progress in the calculations of scattering off isolated atoms; next, some of the issues that we get into when those atoms are not isolated but embedded in various types of environments. We then have the problem of inelastic scattering, which we've also heard a bit about at this conference. In the theoretical discussion we've included some issues of tabulation and parameterization. Also, I will try to say a little bit about what we've heard might suggest for the future.

Now, as far as history goes, we know that this subject began a long time ago. We could trace it back to the ancient Greeks, if we wanted to. But, Thomson, in any event, suggested the possibility of using x-rays to determine the number of electrons in the atom--at that time in terms of his atom, not Rutherford's atom. Barkla, a few years later, about 1905, estimated in that way that there were about half as many electrons in the atom as the atomic weight of the atom. The assumption being made was that you were scattering off all the electrons as free particles, which we call Thomson scattering, or maybe even Compton scattering. Later on, as we know, the work of Compton pointed out that there were inelastic aspects to the scattering of photons off electrons. Meantime, the whole subject of studying atomic structure through elastic and inelastic scattering had begun. You've got a fair review of where that was some years ago in James' book, for instance.

One of the important features was that even a classical description of scattering works fairly well if you assume that somehow the atomic structure is there. Of course, more recently one demonstrated that quantum mechanics did not change the gross details of that description, so that it's been fairly

easy and convenient, over quite a few years, to interpret these experiments probing atomic structure.

Now, when we turn from history to the current status of theory, and begin that discussion with where we stand on elastic scattering, we've heard from two of our talks about a number of the general features that these processes must satisfy. Here, we have Figure 1, based on David Smith's viewgraph, which points out that there are a number of sum rules that are prescribed for both the amplitudes  $f'$  and  $f''$ . The sum rules serve as important constraints on any data set. They can be used, as was shown, to test for discrepancies as a function of the photon energy over large energy ranges.

These particular relations, I might comment, of course, are nonrelativistic relations. So, if you want to go up to higher energies and the highest Z-elements, you will have to be careful. But still, the existence of these constraints has many implications for all calculations, and even for the accuracy of those calculations. We heard another example of that type of discussion in the work of Dr. Freund.

Now, turning more specifically to the case of atoms, we have been discussing here three types of isolated atom calculations. We heard about the calculations done by Cromer and Liberman, quite a few years ago, and about their continued usefulness. They were based, in fact, on ideas of the sort we talked about, utilizing the dispersion relations, and calculations of the absorptive part have generally been treated in terms of photoabsorption. Liberman reminded us in Figure 2 how he made his calculations. He pointed out that there are various problems in the way he initially had done the calculation. There were nonrelativistic assumptions that were made--of course, those can be removed. There are some other things we must be careful about. But, this is a perfectly valid way of determining  $f'$  and  $f''$ , as indeed was described this morning, and it remains a very useful approach.

One then gets into the question of the angular dependence of those terms, because the dispersion approach, in a simple fashion, discusses only the forward amplitudes. While in principle an approach could be written down for finite angle, one must be careful because they would not involve finite angle dispersion relations, but partial wave dispersion relations. (Dispersion relations at finite angle would not be correct.) However, it has become clear that in the x-ray regime, the problem is not too severe. The angular dependence of these extra anomalous terms is not severe, and that can be seen in the Coulomb calculations that Gavrilin has done, as well as in our numerical

NEW DEVELOPMENTS IN OPTICAL SUM RULES

High energy physics ideas and techniques taken back to optics, Phys. Rev. B 6, 4602 (1972)

Refractive index

$$\tilde{n}(\omega) = \epsilon^{1/2}(\omega) = n(\omega) + i k(\omega) \quad (a)$$

$\tilde{n}(\omega)$  is analytic in the upper half plane. As  $\omega \rightarrow \infty$ , a power series expansion yields

$$\lim_{\omega \rightarrow \infty} \tilde{n}(\omega) = 1 + 0 \cdot \frac{1}{\omega} - \frac{\omega_p^2}{2} \cdot \frac{1}{\omega^2} + \dots$$

Analytic function theory ==> moments  $\propto$  coefficients:

- Inertial rule - coeff of  $\omega^{-1}$  term

$$\int_0^{\infty} [n(\omega) - 1] d\omega = 0 \quad \Rightarrow \quad \int_0^{\infty} \frac{f_1(\omega)}{\omega^2} d\omega = 0$$

- f sum rule - coef. of  $\omega^{-2}$  term

$$\int_0^{\infty} \omega k(\omega) d\omega = \frac{\pi}{4} \omega_p^2 \quad \Rightarrow \quad \int_0^{\infty} \frac{f_2(\omega)}{\omega} d\omega = \frac{\pi}{2} Z$$

- Some other rules

$$\int_0^{\infty} \omega k(\omega) [n(\omega) - 1] d\omega = 0$$

$$\int_0^{\infty} [n(\omega) - 1]^2 d\omega + 2 \frac{1}{\pi^2} \sigma(\text{dc}) = \int_0^{\infty} k^2(\omega) d\omega$$

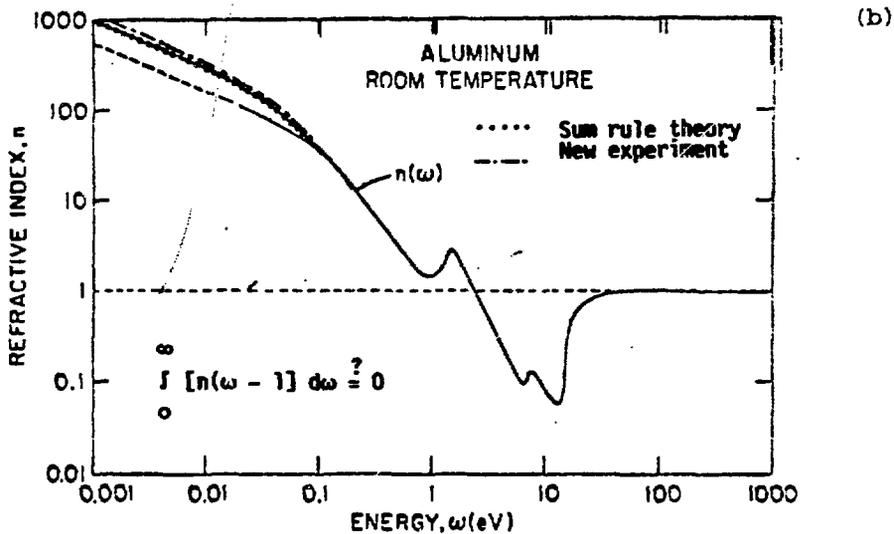


Figure 1. (a) Sum rule constraints and (b) application of sum rule constraints (after viewgraph, David Smith).

$$f = f_0 + \Delta f' + i \Delta f''$$

$$f_0 = e_1 \cdot e_2 \int e^{i(k_1 - k_2) \cdot r} \rho(r) d^3r$$

$$\Delta f' \approx \frac{mc}{2\pi^2 \hbar e^2} P \int \frac{\epsilon^2 \sigma(\epsilon)}{(\hbar\omega)^2 - \epsilon^2} d\epsilon + 5E_{tot}/3mc^2$$

$$\Delta f'' = \frac{mc}{4\pi \hbar e^2} \hbar\omega \sigma(\hbar\omega)$$

$\rho(r)$  is the electron density of an atom.

$\sigma(\epsilon)$  is the photoabsorption cross section.

$\Delta f'$  is approximate because negative energy states are not treated exactly but by means of a non-relativistic approximation.

Figure 2. Basis of Cromer-Liberman calculations.

calculations; Freund has given general arguments as to why that was so. Figure 3 shows Freund's data, with (for hydrogen K-shell) the form factor decreasing with momentum transfer and showing the much slower decrease of  $f'$ .

One can go on beyond this to do a full S-matrix calculation as Kissel described. This is, of course, necessary if you're going up to higher energy, and you will then obtain the information on angular distributions that you care about, effects which are small in the x-ray region. The results which Lynn has presented for forward amplitudes are in Figure 4, which show the type of calculation, the type of results, and the accuracy of the results. In discussing this we should be a little cautious in saying that we see a large discrepancy here. What we see should not be viewed as a statement that the same percentage discrepancy will necessarily apply in regions where the anomalous amplitudes are getting bigger. It may well be more appropriate to say that there is a 0.2 electron unit error in the calculation.

One can also get the angular distributions, and in Figure 5 we have the comparison Kissel showed with the Chipman-Jennings experiment. We also saw in Schumacher's talk some comparisons with his new experimental information on angular distributions. It will be interesting to make a comparison with the experiment of Ice, which we will be looking forward to hearing about.

Of course, no theory is exact and even Kissel's S-matrix calculation should not be described as an exact S-matrix calculation. It is a calculation within the independent particle approximation, describing scattering off electrons moving independently in a relativistic self-consistent potential. One, of course, needs to go beyond that, in many cases, especially near edges. We know various ways to do that from the work on photoeffect, which has developed considerably farther than scattering work, because it is an easier and a less expensive calculation to do. The most extensive such work on photoeffect with systematic surveys over many elements is that started by Zangwill and carried out by Doolen and Liberman in relativistic time-dependent local density approximation. These calculations produced for photoeffect those broad range surveys that, in general, are in quite good accord with experimental data, except for some details near edges, and which merge into independent particle calculations at high energy. As we heard from Doolen, we can now begin to get data of this kind also in the scattering case, for the dipole polarizability and the scattering factor, as shown in Figure 6. I remind you that this type of calculation is becoming available. If it is done as a multipole calculation (these results are dipole and quadrupole so far, I

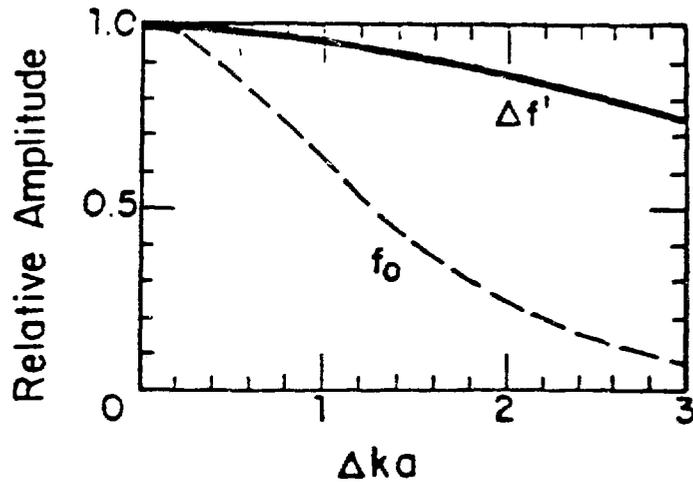


Figure 3.  $\Delta f'(\Delta ka)/\Delta f'(0)$  — and  $f_0(\Delta ka)$  - - - for the 1s state of a hydrogenic atom, where  $\Delta k$  is the wave vector change upon scattering and at the orbital radius, as calculated by Freund.

## f' COMPARISON



17.479 keV (Mo $K\alpha_1$ )	Ne	Ar	Kr	Xe
S Matrix	0.024	0.170	-0.478	-0.416
Cromer and Liberman	0.021	0.155	-0.652	-0.684

22.163 keV (Ag $K\alpha_1$ )	Al	Zn	Ta	Pb
S Matrix*	0.039	0.323	-0.375	-1.034
Cromer and Liberman	0.032	0.260	-0.937	-1.910

\* May 7, 1980, data.

Figure 4. Comparison of 2nd-order S-matrix calculations (Kissel) and the Cromer-Liberman tabulation.

# NOBLE GAS EXPERIMENT



Chipman and Jennings (1963)  
 $^{54}\text{Xe}$ , 17.479 keV (Mo  $K\alpha_1$ )

$\theta$ (deg)	$x$ ( $\text{\AA}$ )	Differential Cross Section ( $r_0^2/\text{sr}$ )				
		experiment	S matrix	%	form factor	%
3.73	4.688(-2)	2.776(+3)	2.763(+3)	-0.36	2.741(+3)	-1.3
4.68	6.608(-2)	2.732(+3)	2.721(+3)	-0.40	2.693(+3)	-1.4
7.31	8.987(-2)	2.623(+3)	2.618(+3)	-0.28	2.487(+3)	-1.4
10.21	1.254(-1)	2.281(+3)	2.266(+3)	-0.68	2.230(+3)	-2.2
14.14	1.735(-1)	1.836(+3)	1.825(+3)	-0.57	1.890(+3)	-2.4
22.08	2.701(-1)	1.388(+3)	1.377(+3)	-0.78	1.348(+3)	-2.8
27.07	3.288(-1)	1.137(+3)	1.125(+3)	-1.1	1.103(+3)	-3.0
32.08	3.893(-1)	9.315(+2)	9.220(+2)	-1.0	8.061(+2)	-2.8

Figure 5. Angular distributions from the second-order S-matrix calculation (Kissel) compared with the experiment of Chipman and Jennings.

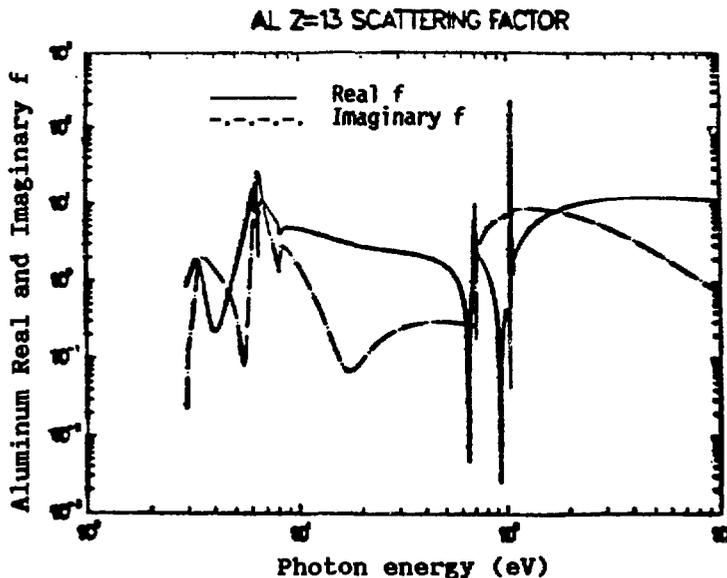


Figure 6. Example of scattering factors calculated in relativistic time-dependent local density approximation (Doolen and Liberman).

understand) by adding the additional multipoles, it would be the next stage beyond the type of calculation that we talked about before.

Now, that may be all well and good, but we have heard from various people (Dudley Creagh and others) saying where is the real world, where are the things that we care about? Of course, the real world is a different place for different people. Nonetheless, it is true that, for many cases, for many purposes, you want to know not about isolated rare gas atoms but about atoms in solids, plasmas, or whatever. That, as we know, is a more difficult problem. We have heard from the solid state side, from Lehr for instance, reminding us of what we can learn from the related process of photoeffect, from EXAFS, etc. Through the connection of  $f'$  and  $f''$  all of that will influence the  $f'$  of scattering theory. We have heard from Koelling about ways to look at the atom in the solid. He, too, was talking somewhat from the viewpoint of photoabsorption, and the point that he was making was that you are dealing with relatively short-range excitations in a long-range structure. He said the way to deal with that problem is to think of imbedded atoms, to think of the situation as an impurity problem. So, he talked about various viewpoints, the imbedded atom, the cluster, super cells and so forth, as ways to deal with this issue.

Now, solids are important, but they are not the only environment, and we did hear a bit about other environments, like plasma environments, which are also of concern. We heard in the work of Rozsnyai, for instance, about how those environments can become more exotic than one realizes simply because of additional processes which become possible with higher temperature. In the work of Liang we heard about some of the direct scattering issues that arise as the plasma becomes hot. He was talking about scattering off foils, which get heated. As a function of time, the number of bound electrons versus free electrons changes, and since it's hot, also the cross sections off those bound electrons may change. All of these things then affect what you see. Questions of: what is the ionization state of plasma at a given moment, what's happening to the absorption edges, what happens due to density effects. Thus, this is another very interesting environment to deal with.

We heard, also, a bit on the photon and electron inelastic scattering problems. In the work of Cooper, we heard how much useful information can already be obtained from the inelastic scattering, and that was also discussed in Platzman's original survey talk. There is not yet, however, a really satisfactory treatment of the Compton effect at the level that we were hearing

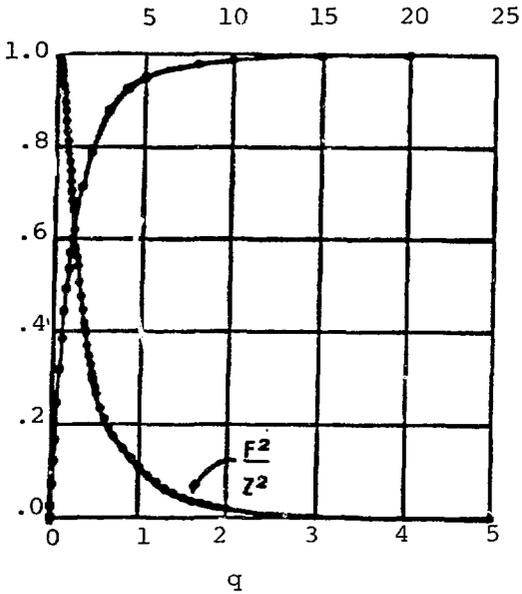
described here for the elastic scattering. We saw in the experimental data Schumacher presented some of the severe discrepancies that still exist, at least in the inner shell inelastic scattering

The next important topic, then, is the issue of tabulation and parameterization. Of course, the classic tabulation in this field has been that of Cromer and Liberman. We also have for  $f'$  and  $f''$  and the actual scattering factors, for the angular distribution and the like, the tabulations of Biggs, Davis, and Lighthill and others. With new predictions that are becoming available there are going to be opportunities to update that type of work, although in many regimes those tabulations remain valid and will be used indefinitely. Figure 7 is an example, for instance, of the Biggs-Lighthill scheme; the curves involve both the coherent and the incoherent scattering factors and show a way for a numerical fitting of those factors which then can lead to convenient tabulations. Another example of that kind we've heard about in the work of More; here the emphasis was on "simple" fast algorithms for large computer codes. So, we heard from More how, in terms of some simplified approximations, they could characterize both the elastic and the inelastic amplitudes. In Figure 8, he, I believe, was emphasizing the total cross sections integrated over angle; for his purpose he had found it sufficient to use some very simplified atomic models, basically fitting the form factors that would enter into his scheme. That led to a very rapid algorithm.

That finally leads us to the question of prospects, where might we be going. In the so-called standard elastic scattering domain, I think it is clear that fairly soon now we are going to have full independent-particle-type calculations available. Thus, through the x-ray regime it will be possible to say what is predicted at that level of approximation for both forward amplitudes and for the angular dependence. I would suppose that if Gary Doolen continues to work on this problem, we will have quite a bit more information on the correlation problem. We will begin to see when those correlations effects matter, presumably primarily for regions closer to the threshold. Over the time scale of a few years, to be more realistic, probably we will understand more about the problem. Some aspects of correlation, of course, are much harder to deal with.

Environment studies are more complicated. You notice that solid state people have worked for a few years on their problems. We will have progress but not final solutions, I would guess. Ditto in the case of the plasma environments, particularly dense environments; we have enough un-understood

Silver (47)



COHERENT SCATTERING

$$\frac{d\sigma}{d\Omega} = \frac{r_e^2}{2} (1 + \cos^2 \theta) F^2(q, Z) \left[ \frac{\text{cm}^2/\text{atom}}{\text{steradian}} \right], \quad q = \frac{1}{\lambda} \sin\left(\frac{\theta}{2}\right)$$

$$\frac{F^2}{Z^2} = \begin{cases} 1 + c_1 q^2 + c_2 q^3 + \sum_{j=3}^9 c_j (q - x_j j_{j-2})_+^3, & q < 2.5 \\ c_{10} q^{-4}, & q \geq 2.5 \end{cases}$$

Figure 7. Parameterization for tabulation (Biggs).

Total scattering

$$\left(\frac{d\sigma}{d\Omega}\right)_{\text{TOT}} = \left(\frac{d\sigma}{d\Omega}\right)_0 \left\{ \left\langle |F(q)|^2 \right\rangle + N - \sum_n |f_n(q)|^2 - \sum_{\substack{n,m \\ (\neq)}} |f_{nm}(q)|^2 \right\}$$

elastic  
or  
"Coherent"

↑  
inelastic or  
"incoherent"

Hydrogenic model for practical use:

$$\psi_n(r) \sim N_n \exp(-r/r_n)$$

$$r_n = a_0 n^2 / Z$$

gives simple, reasonable  $f_n(q)$

we omit  $f_{nm}(q)$  which would be overestimated

set  $\left(\frac{d\sigma}{d\Omega}\right)_0 \Rightarrow$  Klein-Nishina

Figure 8. Simple algorithms for scattering (More).

physics to keep people busy for a year or two yet. There are also other elastic areas like the polarization problems Templeton talked about. Issues of ions can raise quite interesting physics, particularly near edges, because many more resonance type effects become accessible.

Inelastic scattering, I think, is a challenge, and I would love to have somebody help us work on getting an independent particle calculation done for Compton scattering. Resonant Raman scattering and the transition to the two-step process have lots of interesting physics in them, as we heard from Bernd Crasemann. One begins to go beyond simply probing the atom as a semi-static structure and begins to talk about these types of correlated effects and other multi-electron multiphoton effects in the atomic environment.

So, in summary then, I think the prospects for theory are that there is lots to be done; it should be fun for quite a few years yet.

### Questions

Gavrila: I'd like to comment on the situation of knowledge concerning atoms and their environment. After all, the success we have had with the isolated atom is due to the fact that one would integrate the dispersive currents and get into the picture the contribution of the atomic excitations. In the case of the atom in environments, that is actually a crystalline state, what one has thought so far was to calculate the band structure and by Fourier transformation get the form factor. And this is at the level of form factor calculations. What one would like to see is a calculation of the Kramers-Heisenberg matrix element including dispersive terms, with band structure wave functions. In discussing this with Koelling, I am told that that is part of the problem, because it involves a calculation of excited states and at the present time we have a calculation of the ground state by Hartree-Fock or local density functional formalism. At any rate, in order to be able to describe what has happened at the edges, we need a complete first principles approach. This is what is needed and from what I understood, unfortunately, one will have to wait quite a while before one can hope to get that problem solved. So until then, one would have to just use some sort of compromise by considering, as

much as possible, atoms distorted to some extent by the environment.

Del Grande: I would like to say one thing since we mentioned Gary Doolen's photoabsorption calculations using Liberman's relativistic time-dependent local density approximation. The calculations agree very well with our measurements, on the 2-3% level, when we examine measurements in the region of 1 to 10 keV, for eight elements: Fe-U. This agreement is really outstanding. Also, the agreement between the central field one electron calculations, and the local density RPA calculations are also at the 2-5% level. Above one keV, for photo effect, things are working out very well when we compare theory and experiment.

SESSION 3. BASIC EXPERIMENT, REVIEWED

David Templeton, Lawrence Berkeley Laboratory

Roman Tatchyn told us about a novel technique that measured optical properties, at least it's novel to me. That stimulates me to comment that the future directions which will be most exciting, I think, will be the ones that I am not imaginative enough to predict this morning.

A lot is going on in this field. I am sure that other clever people will invent other clever ways to do experiments. At least an important part of the future directions are things that will occur as people invent them. Boris Batterman gave an introduction the first evening which mentioned numerous exciting experiments, some of which were new to me, in both the technical tricks of doing experiments with new facilities and also some of the clever fundamental experiments that meant something of fundamental interest. I'll just cite the segmented bent triangular monochromator, which looks like a very useful technical development. He talked about the time resolved study on the laser melting, which I think is probably a precursor to a lot of experiments. He mentioned the use of time delay to get the Mossbauer radiation, which I think is a very imaginative and possibly very useful technique. Several of the papers talked about the interferometer methods of measuring anomalous scattering. There was one viewgraph from Michael Hart's paper showing a small sample of the very rich results that are coming out of that technique. Ulrich Bonse also showed us some curves by the same technique, in fact for some of the same materials. I think here we need to use the same scale so that we can compare their results. We have two curves for nickel. The two nickel curves, although the scales aren't quite the same, as far as I can tell show excellent agreement. I could show other examples, but to try to move on, I won't.

Creagh showed us some different results, which call attention to this discrepancy at the high energy limit, which he has plotted in a way to make it look most impressive. See Figure 9. These, in fact, are small discrepancies, but the quantities involved are small. His point is that the accuracy of the small effect at the high energy end isn't very good.

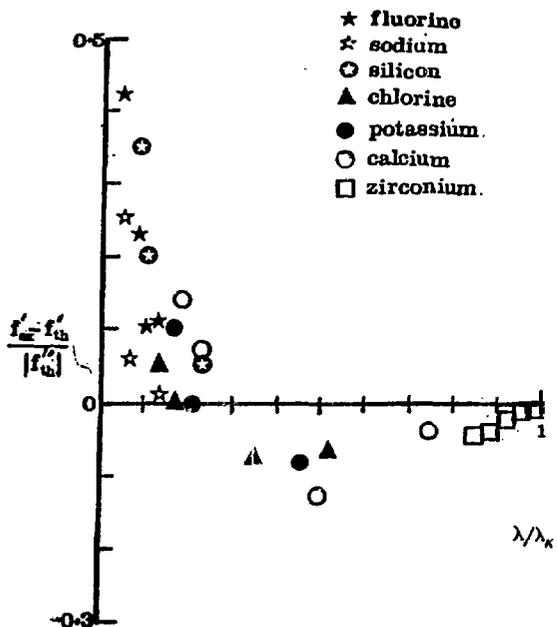


Figure 9. Discrepancies between scattering experiments and theory at the high energy limit (after Creagh).

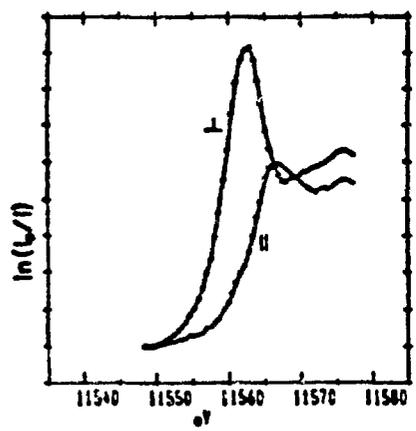


Figure 10. Absorption coefficient (on an arbitrary scale) vs photon energy for polarized x rays with electric vector parallel and perpendicular to the fourfold axis of  $\text{PtCl}_4^{2-}$  near the platinum  $L_3$  absorption edge (after Templeton).

Also, here we have Figure 10, one of my projections, just to remind you that polarization causes very large effects in certain substances. I think there are going to be a lot of interesting examples to study. The effects are not hard to find, if you think about what kind of molecule will show them. They occur almost invariably in EXAFS spectra. I didn't say much about EXAFS spectra, but the polarization effects occur in every EXAFS experiment. I would say that only in a small proportion of the specimens studied do they actually cancel out by symmetry. Most of the substances people are studying do not have the high symmetry that causes these things to vanish, although they often are averaged out because specimens are polycrystalline or amorphous.

Dr. Ketkar reminded us that we are not an island of x-ray physical optics, but that there are other things in the world like electrons. He showed us some results of a very nice experiment involving electron scattering, which, however, can be interpreted in terms of some x-ray scattering properties. Now, I don't understand this very well, but in Figure 11, as I understood it, he has experimental points which agree very nicely with the theory. However, the theory seems to be considered wrong by its authors, who have applied a correction which makes it much worse. This reminds me that there is a folklore, among chemists, that Linus Pauling knew how to construct approximate theories which always got worse when you added correction terms and tried to go to higher order.

Dr. Gaines talked about some of the problems of scattering from real substances. Here is one of his projections in Figure 12 showing various things like Bragg diffraction peaks. These come and go because we are looking at a fixed angle and changing the wavelength: a particular Bragg reflection will come in and go out according to whether the wavelength and the scattering angle correspond. It occurs to me that these Bragg diffractions are occurring in every wavelength; they simply occur at different angles. I think it would be possible to integrate some of these observations and show what happens to the total scattering as a function of wavelength, whether it follows the sum rule or whether the scattering fluctuates erratically with wavelength. Certainly to some extent it will smooth out, because these Bragg reflections will occur at different angles not coinciding with this particular geometry.

We had two very impressive papers, by Cooper and Schumacher, which have been mentioned already by the previous speaker. It is rather presumptive for me to make any deep remarks about this because the authors know so much more about it than I do, but I will perhaps stimulate some discussion by a couple

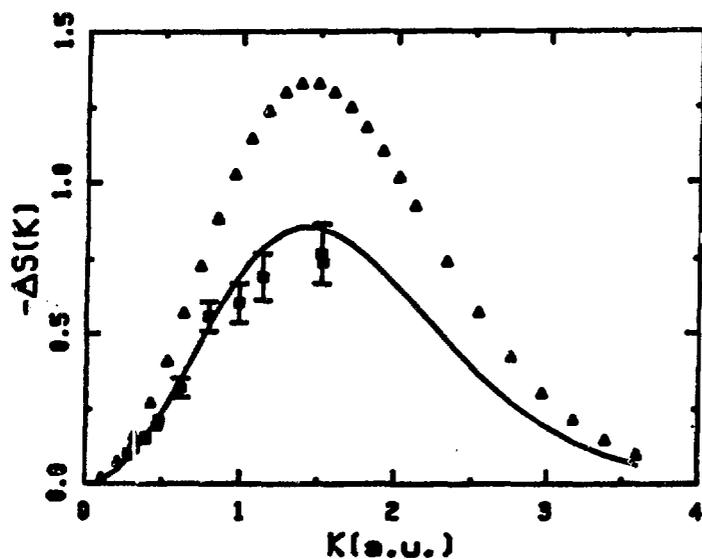


Figure 11. Use of electron scattering experiment to determine x-ray scattering properties (after Ketkar).

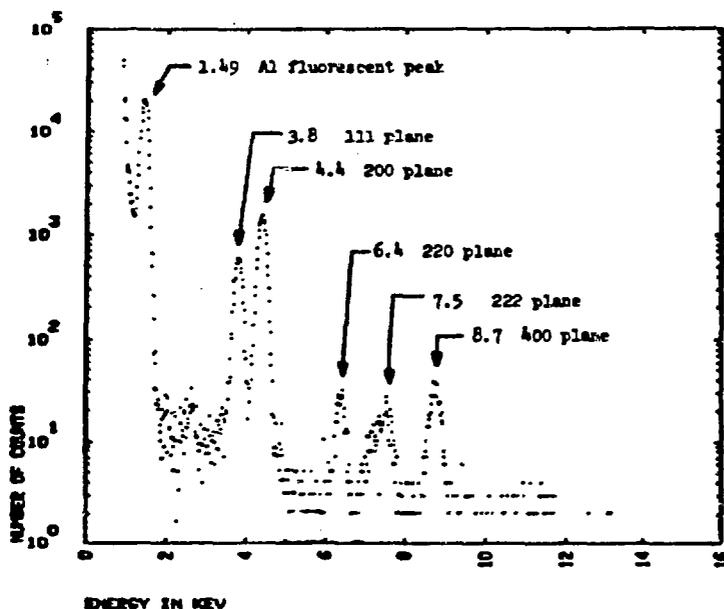


Figure 12. Bragg-like diffraction peaks using an aluminum bremsstrahlung plus emission line source to measure the scattering properties of aluminum (after Gaines).

of remarks. The authors can straighten us out during the discussion period. Here was one curve in Figure 13 where there seemed to be excellent agreement between experiment and theory. There were several other curves of this sort (see Figure 14), which from where I was sitting looked like excellent agreement too, but, Professor Schumacher pointed out that there is a 50% discrepancy that comes from this dense logarithmic scale on the left. Because the phenomena are covering such a wide range of magnitude I don't know whether

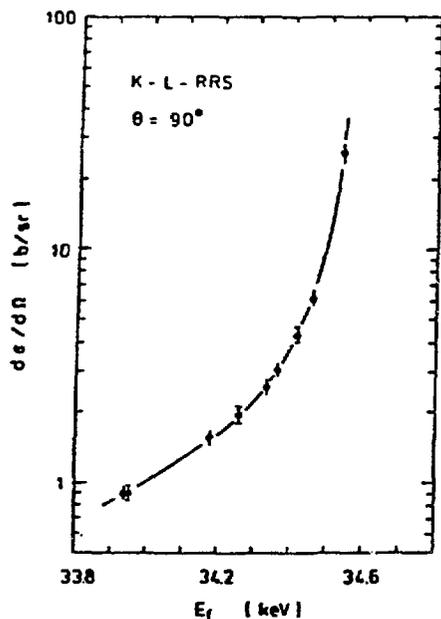


Figure 13. Energy integrals of RRS spectra measured at  $\theta = 90^\circ$  and different primary energies  $E_i$  compared with predictions.  $\circ$  ( $\otimes$ ): scattering plane parallel (perpendicular) to the plane of polarization of the incident photons (after Schumacher).

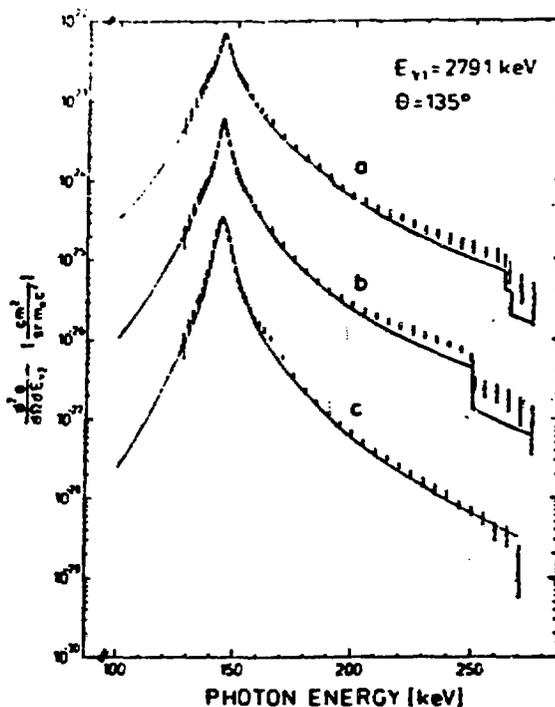


Figure 14. Double differential cross section for the Compton scattering of 279 keV photons by (a) Pb, (b) Sn, and (c) Cu through  $\theta = 135^\circ$ . The predictions of the impulse approximation are depicted by solid curves (after Schumacher).

this is to be regarded as good agreement or bad agreement. Maybe that will come out in the discussion.

I'm running through all of this because I think I could spend an hour and not really summarize the three-hour session, which wasn't long enough for what the various authors had to say. I would like to make some comments about how I see the future of the applications of these results, by people who are doing experiments on real materials. The majority of the current experimental work is close to absorption edges, where things are different. I have a transparency not from the Basic Experiment session. Here in Figure 15 are some measurements we made a year and a half ago on zinc. While metallurgists and solid state physicists have a lot of interest in metals, the typical chemist and every biologist is interested in non-metals. This is a measurement of the imaginary part and the real part of the scattering factor for zinc in the +2 state, in a zinc salt. Superimposed is the Cromer and Liberman calculation. First of all, the wavelength is shifted to make it fit best, because there is a chemical shift of the edge. To go back to the Cromer and Liberman discussion, one of the important things in this business is that it is not always clear what one means by the absorption edge and the photoelectric threshold. These terms tend to be used interchangeably--at least I have the impression they have been used interchangeably--but, in fact, the photoelectron threshold is at higher energy. These big resonances that occur at the edges, this one in particular, certainly is at least principally to bound states, not to photoelectron states. A lot of applications are in this range where we're not making photoelectrons. The experimenters are not going to wait for the slow progress of theory. I challenge and encourage the theorists to do calculations about what is happening in these different chemical states. But, even if I am successful in stimulating theory, the experiments are not going to wait. The experimenters are going to run ahead, and they are going to use these values whether they have been properly calculated or not.

Let me show a curve for zinc metal, Figure 16, from Hart's lecture. There is a resonance line, but not very large. In Figure 15, the resonance line is more than double the edge jump. That's the difference between the metallic zinc and the ionic zinc.

I see the interferometric technique as a method of choice to get really reliable accurate experiments on  $f'$ . As was explained quite clearly, the Kramers-Kronig integration of these will give reliable values of  $f''$ , given a

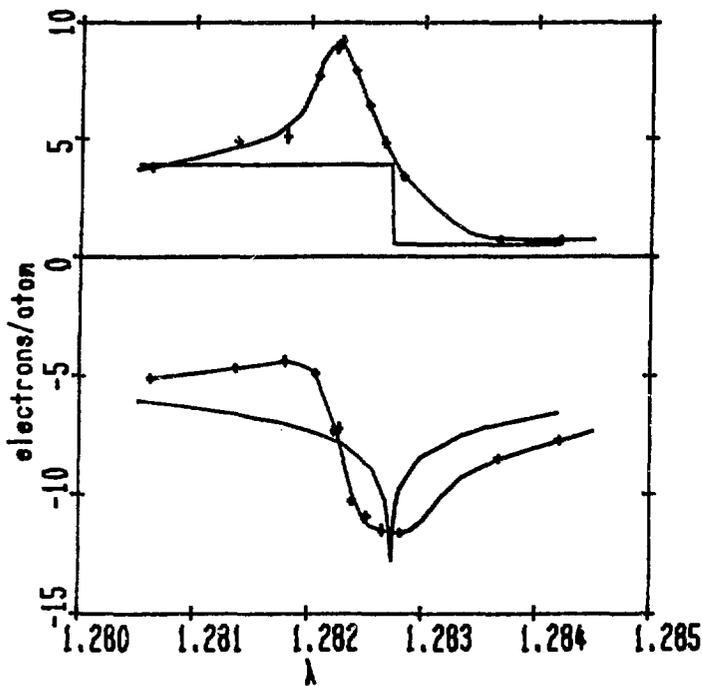


Figure 15. Anomalous scattering measured for  $Zn^{2+}$  ions, compared with Cromer-Lieberman calculation (after Templeton). Editorial note: the big resonance that occurs at the edge for zinc was a subject of discussion following the session.

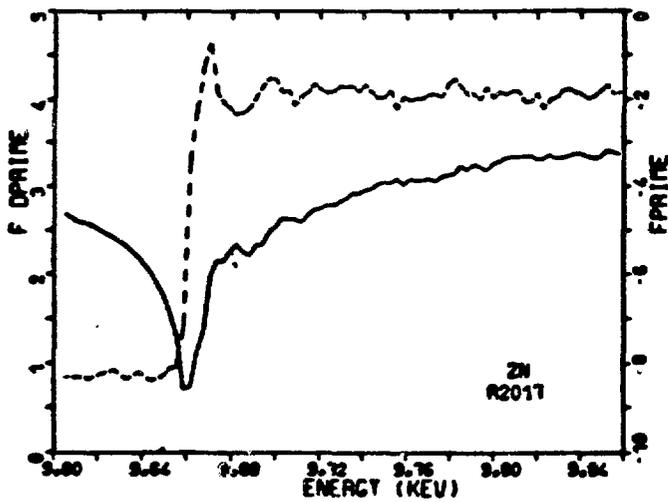


Figure 16. Anomalous scattering measured for metallic zinc, after Hart, shows a smaller resonance line than was shown for ionic zinc by Templeton.

sufficiently wide range of wavelengths. It's also clear that the present state of theory is quite good at some wavelengths remote from absorption edges. There has been a lot of criticism of trying to derive these things from simple absorption curves. The theorists present here probably don't know the full story about how bad the experimental problems are. A lot of these curves are wrong, for reasons that are well known but not always advertised by the experimentalists. In particular, it is very difficult to get the absolute scale. It is a powerful method to get the shapes of the variation. And in most of the derivations, when an experimentalist says he gets it from the absorption curve, what he means is he measures an absorption curve on a scale which he didn't even bother to write down. He didn't weigh the sample, he didn't measure the thickness, but he notices it absorbing x-rays and the logarithm of a ratio is so much. Those are scaled by believing somebody's table, Cromer-Lieberman because it's the one that's accessible. If any one else wants to supercede Cromer-Lieberman, they've got to write an extensive table or a convenient code that people can run to get the numbers. A typical experimentalist doesn't care where the theory came from or what it means, he only wants an answer that he can use as a security blanket to scale his absorption curve.

Professor Bonse showed us that the interferometer technique can observe the polarization effects, if you have a suitable specimen. The interferometric technique suffers still from one disadvantage. You must have a suitable specimen. Suitable specimens are easy to get for some materials. It is possible to get them for many materials, but only if one knows their properties and knows how to prepare them. There are many interesting substances for which I think it will be impossible to get adequate quality specimens for interferometry. So, as I see the future, the experimentalists are going to measure absorption curves, and they are going to fit them on to what they can get in the way of new tables, and if it is done properly, it's an excellent way to get  $f''$  through the absorption region.

The way they will get  $f'$ , if they are smart, is not to attempt to do the integral from zero to infinity. They will do the integration in a limited region, having scaled their spectra at both ends to reliable values. Instead of integrating  $f''$ , they will integrate the difference of their absorption curve from, let's say, whatever one calculates with Cromer's program. These integrals are convergent; you don't have to worry about what you do with the

infrared and gamma-rays limits, if you are only integrating the difference between these two curves.

I can't close without mentioning out that there is still a fly in the ointment, which was pointed out in the very interesting talk about the sum rules. When we modulate this spectrum with all this rich structure at the edge, we may put in more oscillator strength; we may take out some oscillator strength. If you change the oscillator strength it has to go back somewhere else. A very important question for the theorists to explore is where they think it goes. That's crucial to the assumption that in my zinc+2 ion, that is the only thing different between the ion and the isolated atom of neutral zinc (which is actually not even zinc metal, but a zinc gas, within the theoretical calculations). I would like to know how good it is to assume that my experimental curve with edges really matches on to the theoretical curve (below 1000 eV away).

Rather than take more time, I'll stop and hope there is some discussion.

### Questions

Cooper: I would like to make a couple of comments, one in response to the query you raised about the absolute magnitude of Compton scattering. I actually don't think there is a very significant discrepancy, although I'm not sure whether Martin would agree with me or not. Because in order to place those things on an absolute scale you have to work very hard at the multiple scattering corrections and things of that kind. My feeling, from having banged my head against that particular wall for quite a long time, is that you may well finish up with errors in details. There are other problems in high-Z materials, like bremsstrahlung, which we haven't really delved into very deeply. If I could just make one comment from the point of view of Compton scattering studies of ground states, the area that I see exciting interesting things coming along is an area that can be opened up if some of the clever people here designing the synchrotron facilities can give us a reasonable intensity of circularly polarized radiation. Unlike diffraction experiments, we need the radiation circularly polarized rather than linearly polarized to pick up the spin effects. Still, the

only way this has been done so far has been by using very weak Mossbauer sources. But if somebody can tell you over the next 10 years that we may have from crossed undulators, or whatever, circularly polarized radiation with an energy of at least 25 keV, then that will make me very happy indeed.

Del Grande: I have a question on zinc vapor versus zinc solid. I would be very interested in seeing the data to learn if some comparisons could be made regarding the near edge structure for the vapor and the solid. There seems to be a 10% effect in photo-absorption, anyway. Do we understand this? There seems to be a 10% enhancement of zinc photoabsorption cross sections when one averages over the near-edge structure. I think this applies to both the vapor and the solid.

Templeton: Let me clarify, there are experimental data on zinc metal, there are experimental data on zinc+2, and this is just one example of what occurs almost everywhere in the periodic table, that you change chemical state, you change these edge spectra. The zinc gas was a comment on the theory, when you do atomic physics calculations on the zinc atom, a chemist says that is a gas, simply because only in the gas do you have isolated atoms. So, gas is just a chemical name for one atom without any neighbors. Now, zinc has a vapor pressure that is significant enough that I think it is quite practical to do an experiment on x-ray absorption in real zinc gas by using a furnace and a long tube, but I don't know that anyone has ever tried to do it.

Del Grande: What I was mentioning applies also to argon, which presumably is like the atomic situation, where you have that same enhancement right above the edge of argon and above the edge of most materials through zinc. There is a 10% difference between what theorists calculate and what we measured. I was wondering if you had any explanation.

Templeton: Well, I've got an idea, a very simplistic chemist's idea of those wiggles in gases. The continuum density of states is a

nice smooth function in a box without any perturbations. But this box that the atom is in is perturbed by the distance from the atom, and I don't think that the density of states in the continuum is the simple particle-in-a-box density. It is perturbed by the existence of the atomic potential. It is clear, at least in argon, that some of the experiments are resolving or partially resolving the transitions to the discrete states of the atom, but the nearby continuum certainly adds some modulation to that atomic potential.

Schumacher: I first wish to say thank you for this comment on the Compton scattering data. One, of course, has to be suspicious about putting things like this differential cross section on scale, and one has to be suspicious about the correction for bremsstrahlung, but in parallel with our scattering experiments we had a separate project by which we tried to investigate bremsstrahlung and we did not publish these things before. We assumed we were sure, or thought we were sure, that things were correct. So, there is hope we published correct things. That is one point. The other is that the Whittingham type of calculation, that means calculations based on the second order S-matrix, suggests that there should be a discrepancy of the same size, maybe 50%. So, the Whittingham type of calculation finds the discrepancy holding in half of the energy spectrum, and there is a disagreement with the experimental finding at the upper end of the energy scale. That should be a good reason for Professor Pratt and his group to do a decent calculation. After that we can see whether or not we really have a discrepancy.

Kim: I hope to answer Dr. Cooper's question about circular polarized radiation at 25 keV. Until this conference I was rather modest about the capability of cross polarizers for producing circular polarization at high photon energy (about 10 keV). But now I am more hopeful. I'm convinced that this technique of producing

circularly polarized radiation through crossed undulators will be capable of indeed meeting Dr. Cooper's requirement. I think for 10 keV to 45 keV certainly crossed undulators placed in synchrotron sources like the 6 GeV machine should be able to produce a degree of polarization of 20 or 30 percent. But it is of a variable type.

Templeton: Yes, I think it is very clear that the modulation of polarization is essential.

Creagh: I think that what Nancy was referring to is a general trend up from the extrapolation of the photoelectric curve, in order to put it through the median of the EXAFS curve. (Editorial note: see Figure 17.) EXAFS in single scattering approximation is a sine wave. People like Dryer and his workers, however, have found it necessary to put in a linear term.

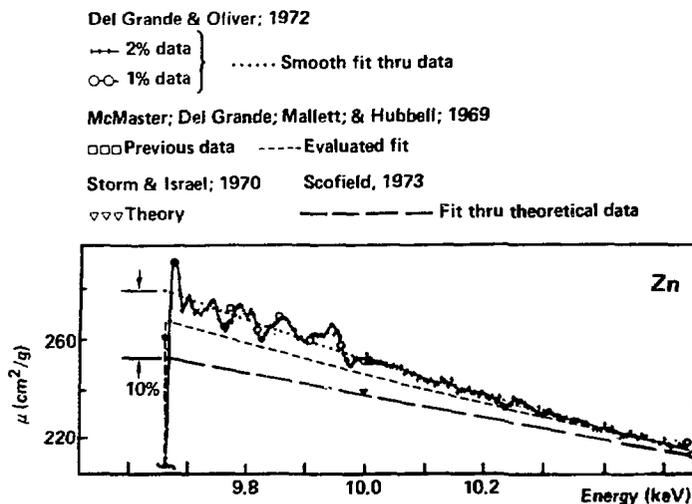


Figure 17. Precise attenuation coefficients show enhanced behavior for metallic zinc having a broader energy range than near-threshold effects, suggesting a 10% enhancement of attenuation coefficients above IPA (independent particle approximation) calculations (discussed by Del Grande).

SESSION 4. WHAT LIES AHEAD, REVIEWED

George Brown, Stanford University

Predicting what lies ahead in the field of x-ray scattering is both a hard and an easy job. It's a hard job, because no matter what insight one brings to bear on the results that have been presented at this and other conferences, effectively, the most exciting things to happen in the future are just glimmers in people's minds today. We will only hear about them a few years from now. It's an easy job, however, because hopefully, I'm not going to be held too accountable for those things that I overlooked. I will try to extrapolate, therefore, the results that were presented at this meeting and at some other meetings that I have been to, from where we presently stand into the near future. I will venture five or ten years into the future when I get a little more speculative.

Let me begin first with the discussion of x-ray sources, which is, of course, leading to the future of the experimental programs. I think it's altogether appropriate now that we refer to electron storage rings as conventional sources of x-rays. There are enough of these facilities now, in existence and in operation, and they are well enough understood, that we can refer to them now as classical radiation sources. At the NSLS, for example, there are under development a number of new high-intensity beam lines, a scattering beam line, which unfortunately, was not discussed at this meeting; a high x-ray energy beam line that will be illuminated by electrons circulating through a superconducting wiggler. There will also be, as I understand it, a beam line on the 0.5 BeV machine that will be dedicated to holography and microscopy experiments. These are very exciting new sources of high brilliance photons at the NSLS that will stimulate a lot of new research ideas. At Stanford an undulator beam line is being constructed for the "so-called" beam line wonder, which is a collaboration among several institutions (Xerox, NSF and SSRL) which will have an interchangeable set of undulators to provide a continuous tunability of photon fundamentals from some 200 electron volts to a kilovolt. This is a very exciting technique that will enable the soft x-ray and vacuum ultraviolet community to be able to cover a

wide range of photon energies with a single beam line, and with extraordinary intensity.

SSRL is constructing a scattering beam line, again, very much like the scattering beam line being constructed at the NSLS; a very high-intensity, general purpose beam line, whose activities will be focused on x-ray scattering. Then there is a set of beam lines, a complex of bending magnet and wiggler-illuminated beam lines being constructed by a consortium consisting of the Lawrence Livermore National Laboratory, the University of California system, and SSRL. A lot of very new and exciting capabilities will be added to the Laboratory when this project is complete, and I might add these facilities will be available not only to these institutions, but to the general user community. At SSRL we are developing the beam line, in fact the first x-ray undulator beam line which will provide x-rays of very high spectral brilliance in the wavelength region in the neighborhood of 1 Angstrom. Then, we have the more speculative storage ring source, the proposed advanced light source at LBL, the advanced x-ray laboratory for want of an official name, the proposed 6-GeV electron storage ring.

These projects will be very crude, perhaps five or six years from now; I think that they will be providing, besides high-intensity, linearly illuminating polarized radiation; they will be providing the circularly polarized radiation that is so useful in the kinds of experiments that have been discussed at this meeting. I might add parenthetically, by the way, that this issue of circularly polarized radiation that has been demonstrated by Carl Chamberland and coworkers that quarter-wave plates are achievable at x-ray wavelengths using basically Laue diffraction through perfect crystals of materials. So, it is possible to transform linearly polarized radiation into circularly polarized radiation and vice versa. A technique that will prove useful, I believe, well before these ultimate sources of variable polarization are available.

The more speculative sources, which consist of the free electron laser and the transfers off of the Klystron were mentioned by Dr. Kim. The proof of principle of the free electron laser has been established. That is, free electron lasers have now been successfully operated with nonvanishing gain. The ultimate gains in intensities, however, I believe are uncertain because of technical problems that are still unresolved. These problems include the fabrication of mirrors that can handle the intensities required, and also, the problem of the delicate interaction between the electron beam and the

undulator magnitude, which has not been completely resolved. So, time will tell how practical these sources are, ultimately, as radiation sources.

Finally, with relative sources, of course, Dennis Matthews gave a very nice presentation of the principle of a material laser at 200 Angstroms, a very exciting development. This is undoubtedly the world's brightest source of 200-Angstrom radiation. The peak power that they observed was 500 watts over periods of time, 250 picoseconds. Already this instrument is ready for experimental research. Although it is the brightest source of 200-Angstrom radiation in the world, in some sense it is also the weakest source. It's average power is three picowatts. It's not going to be competitive for a while with synchrotron sources for the classic experiments where the total number of photons matter. But it will be really useful for those experiments that depend upon peak intensities such as damage-limited experiments, where some kind of chemical process initiated by the photon beam chews up a sample, so to speak, and where you would like to have all the experiments take place as rapidly as possible so that other time constants don't ultimately ruin the sample. And, of course, for time-resolved experiments, 250 picoseconds is a very short period of time, and the kinds of intensities available in that 250 picoseconds are just not available for synchrotron or conventional sources.

What can one say in general, as we proceed to develop higher intensity sources? We can generally say that we can study with greater precision the time evolution of physical processes. Of course, we heard a very nice presentation in a subsequent session about time-resolved experiments both at the nanosecond, the microsecond, and the millisecond level. And we will be seeing, I think, a great deal of activity in this field. There has already been a lot of activity in the biological community, particularly the Hamburg study of biological systems. I think this is a very exciting frontier. As Art pointed out, if this arena progresses as people think it might, I think we are going to be inundated by biologists and chemists who will begin to dominate the synchrotron radiation and x-ray scattering search. Furthermore, we can proceed to study progressively lower and lower Z systems. That is to say, the two-dimensional systems, for example, that have been studied in the past always started with a relatively heavy element such as krypton. It is no accident that that is the case, and that the process would proceed down the periodic table from krypton to argon to neon, and I believe, ultimately to dealing with hydrogen. I don't think that it is out of the question that

people will begin to study the critical phenomena in two dimensions on the lightest of elements: hydrogen and helium.

Low concentrations are an obvious frontier. And, of course, low concentrations would be generically, perhaps, surfaces or biological materials. It turns out that most biological systems and metals of interest are present in very low concentration; concentrations well below those that are generally achievable. The more concentrated elements are just within the range of present day techniques. As the intensities increase by an order of magnitude, the number of compounds of biological interest, for example, will increase by well more than an order of magnitude. Resolution is going to be the frontier that will enable the scattering communities to study correlations of matter at relatively large distances through the scattering process, rather than through imaging methods. That is, we now can see the results of experiments where the angular resolution is one part in  $10^4$  where correlation distances are being studied of the order of one micron or so. The brighter synchrotron sources are essentially sources that don't have more net photons in the beam but have those photons concentrated within a narrower angular volume. That narrow angular volume allows us to study through the scattering process larger and larger areas on the order of 10 to 100 microns referred to as techniques of microscopy. There is a large effort taking place in the United States and abroad to use soft x-rays as prompt synchrotron sources of illumination for microscopic methods. This community is just on the threshold of being competitive with electron microscopy, not so much in terms of spatial resolution, but in terms of doing interesting biological research. Progress has been so rapid that I expect that within two or three years resolutions on the order of 200 Å will be achievable in living samples. This will be revolutionary to the biological community.

These are the general frontiers that undoubtedly will be the directions in which the research will go. I would like to say a little bit about electron spectroscopy. Commenting on the material presented by Professor Crasemann, the gas phase threshold spectroscopy, for example, will be of extraordinary experimental interest now because we can probe the details of the threshold excitation process. We can tune the photon beam continuously with high resolution through an absorption edge, and we have a whole arsenal of spectroscopies that can tell us how the atom is reacting and relaxing from this pinpoint excitation, if you like. Already, we have very nice results on

the threshold excitation of rare gases. This has stimulated the development of theories which treat in a unified way the photoexcitation process.

Our theoretical understanding of the elastic scattering process and the high brilliances available from synchrotron sources are spawning a revolution in conventional crystallography. We are achieving a higher accuracy now in the measurements of the crystal structures of proteins, for example, because the radiation damage problem is greatly reduced by the advent of high intensity sources. Probably most of the people in this audience are familiar with this fact, but for those who aren't, what is important here is that experiments with protein crystals generally are limited in their information content literally by the destruction of the sample from the photon beam. But this destruction of the sample generally takes place by the migration of radicals through the crystal in the aqueous medium that percolates between the unit cells. And, therefore, it is a time-dependent phenomenon. If you can illuminate within photons a sample for a shorter period of time you can gain more scattering information per unit photon. That is, you can achieve the data set before the sample is reduced to ashes. This has already proven to be a boon in the field of protein crystallography.

Anomalous scattering, of course, is now coming of age with the understanding of many of the complex effects associated with the scattering at resonance. The Templetons have pioneered the experimental study of this. High linear resolution experiments are, of course, now ideally matched to the high brilliance sources. Small angle scattering experiments with high resolution about the reciprocal lattice spectrum are very actively pursued at, I believe, all of the national laboratories.

Regarding inelastic scattering, you've heard from several different speakers. Many of the applications of inelastic scattering or Compton scattering relate to the excitation of plasmons in solids. The use of inelastic scattering to determine the band structures of solids was not discussed in too great a detail in this meeting, but I believe it's an exciting new frontier that will be of great interest and you will see a lot of activity with the high brilliance sources. We heard from Dr. Hastings about the higher resolution techniques that will enable us to do phonon spectra of materials that have inconvenient nuclei, which are very small, or for which one wants to study surfaces. All these domains are inaccessible to neutron scattering. Then, of course, there is the magnetic x-ray scattering which has already had exciting results which have been presented.

One of the subjects that I believe is going to be studied with very great vigor over the next few years is photochemistry, the process of taking a photon beam and using it to initiate chemical reactions in a selective way. Already there have been preliminary experiments along these lines, and of course, there is a very extensive body of knowledge already on photon-stimulated desorption, a technique which makes use of the tunability of these bright sources of radiation for selectively desorbing particular species of interest.

Finally, I want to comment on what lies ahead for the nuclear resonance methods. Dr. Hastings discussed the Mossbauer effect and the possibility of resonantly diffracting x-rays from synchrotron sources by nuclei of selective elements. This, I believe, will spawn a renaissance in Mossbauer spectroscopy because it will provide us with very highly collimated beams of very highly monochromatic photons. That's obvious enough. It will also give us a window on a new phenomena, one that has been observed by the Soviets and has long been predicted, the phenomena of nuclear super radiance. This is now a classical subject in the case of atoms. It is the notion that you can speed up the decay of nuclei by exciting a regular lattice with photons, or the possibility of holography with synchrotron radiation by using these photon beams that have meter-long coherence lengths. I think this is something that will be explored over the course of the next few years. Finally, on a more speculative note, again with photon beams that are so highly monochromatic, it is now possible to imagine doing a much better job, for example, of measuring the gravitational red shift. This experiment was previously limited by the brilliance of the angular collimation of the photon beam. The synchrotron radiation from what is now conventional synchrotron sources is many orders of magnitude more intense than the conventional Cobalt 57 source. If we can figure out techniques of filtering out all of the noninteresting radiation, we could improve on this experiment by perhaps an order of magnitude or so.

SESSION 5: APPLICATIONS, REVIEWED

Paul Fuoss, AT&T Bell Laboratories

Last night and earlier this week we heard from a variety of speakers, many of whom have either touched on or spent a lot of time discussing applications of x-ray scattering in dense matter physics. This is a very broad area of research. It involves studying very, very subtle processes. It's essentially impossible for me to review in 20 minutes the details of these experiments. So, I hope that you paid careful attention during the original talks, because I will not say very much about the exact details. I will try to summarize briefly the talks that we've heard.

Tuesday night, Phil Platzman gave a talk on the phenomenology of scattering processes, including magnetic and inelastic scattering. He pointed out that it has been well understood for at least 15 years that you could learn a great deal of information about processes in condensed matter systems by looking at the inelastic processes. But, very little has been done along this line primarily because of difficulties with the technique. Recently, the x-ray sources have been improving to the point where we hope to be able in the near future to make significant progress in understanding inelastic scattering. This would lead to our understanding of electronic and other collective effects in condensed matter systems.

I will also discuss the use of magnetic scattering, which has been a topic of a lot of interest recently. Bob Batterman gave an overview of experimental capabilities and prospects, especially at CHESS. He discussed how we can produce lots of photons, put them on a sample, and use them efficiently.

Last night we had a variety of much more specific talks on specific techniques. Brian Stephenson talked about three different experiments looking at time dependent, time resolved, x-ray scattering. One experiment he discussed was done by people from Oak Ridge and CHESS looking at the melting of silicon surfaces during laser radiation. He talked about some experiments which were being done by the Bell Laboratories by Dennis Wong and Dave Ackley and others looking at phase transitions involving ferro-electrics. And finally, he talked about his own research looking at phase transition in amorphous materials. By looking at experiments, in situ, at elevated temperatures, you learn much more about the details of the phase transition

than you do by the classic techniques of taking a sample, punching it, and looking at a static structure.

Jakob Bohr talked much more about magnetic scattering. In particular, he talked about the study of holmium. In this study you see a variety of very subtle effects going on with magnetic moments. I think it is a very beautiful experiment that shows the power of using x-ray scattering in magnetic studies.

Sean Brennen talked about the area of surface x-ray scattering. Because of the high brightness of synchrotron sources, the use of x-ray scattering has been extended to looking at monolayers on surfaces. In these studies we see results very clearly and cleanly, studying the structure of layers on surfaces and looking at the melting transition, for example, which goes to a high level disordered state. The hope is here that surface x-ray scattering may become the standard technique for studying the structure of surfaces and bring to the field of surface science the technique with all the power and beauty that x-ray scattering has brought to bulk condensed matter systems.

Jerry Hastings talked about inelastic x-ray scattering measurements, in particular Mossbauer work that George was mentioning, and also, backscattering methods for producing very monochromatic beams and analyzing, with a high degree of energy resolution, the inelastic scattering materials.

Finally, Karl Ludwig talked about an x-ray anomalous scattering study of liquid  $\text{Ge Br}_4$ . This study was a test case of a technique which is now in wide use, particularly at SSRL, to study a wide variety of assorted systems, for example: amorphous materials, liquids, and some biological systems.

This is a very broad range of topics that we get out of five speakers. If we chose another five speakers at random from the community of people using x-ray scattering to study materials, we would probably get a totally different set of five topics, and this could go on for some time. It is a very broad field, impacting a lot of areas. For example, these are all topics looking at condensed matter physics, and you have another entire huge field in biological materials and chemical materials. The range of these techniques is just astounding. This has greatly excited the scientific community. Now, I am going to diverge from reviewing what went on last night in order to talk to you a little bit about the general field of x-ray scattering.

The first thing I would like to say is that today's experiments are aimed at understanding very, very subtle effects. Magnetic scattering effects that Jakob Bohr is looking at are processes that happen at not 1% of what we traditionally look at. They are effects that are happening at  $10^{-6}$  of the

electronic scattering effects. That is sort of the general trend in application of x-ray scattering today. These people are looking at more and more subtle phenomena. Another place that you would see the same sort of effect is in x-ray scattering from surfaces. This gives an extremely weak signal compared to the fault and time resolution. While you have the signals at large, you're trying to make the measuring times shorter and shorter. Today's experiments are aimed at understanding very subtle effects. There's a great deal of excitement about this because it is possible to measure these very subtle effects using today's synchrotron radiation sources and to relate them to very elegant theories describing condensed matter. The reason that there is so much excitement about this is because the capabilities are rapidly changing.

You heard in Phil Platzman's talk that the ideas of doing inelastic scattering have been around for 15 years, but the sources haven't been around. One big change is that the NSLS is coming on-line. While many of these techniques have been tried at places like SSRL, the huge number of beam lines coming on-line in this year, and in the next couple of years, should allow the routine implementation of these techniques that have been discussed widely for the last 10 years.

Furthermore, wigglers and undulators are coming on-line; for example, at SSRL this year we should have, as George Brown talked about, an undulator on tap which will move the NSLS kinds of capabilities such that the NSLS will be another order of magnitude brighter. Hopefully, this will allow these techniques to be expanded into new regions.

Finally, I would like to comment, that as George talked about, there are new source developments. And these developments may allow the development of techniques which are currently crackpot dreams. This is why I don't think George can be expected to predict them. But, today's crackpot dreams may be tomorrow's experiments. Unfortunately, when you have a conference like this it has another implication, which is that we didn't hear about great future experiments because none of us are currently crackpots!

## Session 6A

### X-RAY OPTICAL TECHNIQUES, REVIEWED

John (Hal) Mallett, Lawrence Livermore National Laboratory

As we have noted several times during this workshop, this is truly a renaissance period in atomic and x-ray physics. Many of the advances in theoretical and experimental x-ray scattering have been described during this workshop, including some of the advances made in x-ray optics as discussed in Session 6A, "X-Ray Optical Techniques."

The development of x-ray beam lines on the synchrotron facilities around the world has provided us with an extremely valuable research tool for exploring x-ray optics in much greater detail than has ever been possible. It is now practical to have narrow band, continuously tunable, very high intensity x-ray sources, which are necessary for scattering experiments. Much of that capability has been made practical by virtue of the progress made in x-ray optics, particularly during the past decade. Thus, we see a very beneficial synergism and a "bootstrap" effect in the development of two seemingly unrelated fields.

The three papers given in Session 6A dealt primarily with experiments that would lead to a better understanding of dispersion elements/diffraction crystals as a direct application of experimental x-ray scattering.

Henke described the theory and calculations of a series of experiments that ranged from scattering from isolated atoms to the effect of scattering from ordered atoms and molecules such as found in natural crystals and the variety of man-made "crystals". Typical experiments measure the integrated reflectivity of the crystal as a function of energy and relates that to a calculation such as given in the Darwin-Prins theory. The integrated reflectivity at each energy is measured by integrating the experimental diffraction line produced by varying the angle theta.

Kortright described a proposed experiment to probe the atomic scale structure as a function of depth of the layers in a multilayer and interfaces between them. These relatively new, man-made multilayer structures which are produced by depositing thin alternating layers of materials having large electron density differences have been shown to behave as diffraction "crystals" in the Bragg geometry. Kortright suggests combining the ideas

behind the standing wave fluorescence technique (after Batterman, Golovechenko, and others) with a geometry similar to that of the grazing incidence scattering technique (after Eisenberger, Fuoss, and others).

Kvick described a facility which has been established at the NSLS for conducting research in crystallography. Designated the Crystallography Beam Line, X-13B, the facility provides virtually all the needed support to conduct high-resolution ( $2 \times 10^{-4}$ ) experiments over a wide range of wavelength (0.6 to 3.1 Angstroms). Combining the best of the parameters available from the monochromator with the time structure of the synchrotron micropulses should allow time-dependent studies (e.g., electric field excitation), charge density studies (organometallics), and experiments on microcrystals down to one micron (as zeolites) or on macromolecules (such as viruses).

Session 6B

PANEL REVIEW OF SESSIONS, CONCLUDING REMARKS

John (Hal) Mallett, Lawrence Livermore National Laboratory

I don't know about you, but I'm tired. But, if that is a measure of success of an activity like this workshop, then I hope that you are tired too. I feel good about what has happened during the last three days. We have come a long way in those three days. We have had a lot of good food, a lot of good wine, but mostly a lot of good physics. And that's what we're here for! There was some worry about whether one could do good physics in a pleasant environment like this. I think that we showed that that was not an issue.

Carl Poppe in his opening remarks commented that this is a prime time for scattering, and this is an exciting time for physics. I think that was borne out as we could see from this morning's summary of the papers we've had the last few days. Clearly, x-ray scattering is not a dead area like it was 25 years ago, as was shown in one of the slides that we had. Twenty-five years ago there were zero papers on x-ray scattering in the literature. Now there are upwards of one hundred per year.

We in L-Division at the Lawrence Livermore National Laboratory had a number of objectives at the outset of this workshop. We saw this as an opportunity to get theorists and experimenters together, and perhaps even talking to each other. I think that actually happened. Our motives weren't totally altruistic, however. These workshops cost a lot in terms of people, time, and money. We feel like this workshop has been a good investment. It gave us a meaningful survey of the area, in the cheapest way possible, by gathering together what each of us consider to be the resident experts in areas of x-ray scattering.

We hope some day to return our thoughts to physics research in L-Division; something we haven't done in a number of years now. Workshops like this will help us to decide where to put the limited resources that we will have. As many of you are aware, we had a workshop here a year ago on soft x-ray photoabsorption, which was also quite successful. There is certainly one observation that I can't help but make between the two workshops. "Scattering" people drink a lot more wine than "photoabsorption" people. I would like for

you to join me in thanking the organizers of this workshop, especially Nancy Del Grande, Richard Pratt and Jan Meamber, our registrar, for putting on this very successful workshop.

#### ACKNOWLEDGMENTS

R. Pratt (Pittsburgh) was the chairman of the committee that developed the workshop program; the other committee members were A. Bienenstock (Stanford), R. Bonham (Indiana), B. Crasemann (Oregon), N. Kerr Del Grande (LLNL), P. Ebert (LLNL), M. Gavrilu (Amsterdam), B. Henke (Hawaii, LBL), D. Liberman (LLNL), D. Templeton (LBL), K. G. Tirsell (LLNL), and A. Toor (LLNL). An organizing committee, chaired by N. Kerr Del Grande, planned the workshop; the other members were W. Cooper (LLNL), J. H. Mallett (LLNL), J. Meamber (LLNL, Registrar), and C. Poppe (LLNL).

PMB/

## APPENDIX A: PROGRAM SCHEDULE\*

### New Directions in X-Ray Scattering Workshop

Session 1. Opening Session: "Overviews", Tuesday evening, 7:30 p.m.

John (Hal) Mallett, LLNL - "Introductions" (3)

Carl Poppe, LLNL - "Welcoming Remarks" (5)

Nancy Del Grande, LLNL - "Announcements" (3)

Chair: Richard Pratt, University of Pittsburgh

- 1.1 Boris Batterman      Overview of experimental capabilities and prospects (45)
- 1.2 Mihai Gavrilă      Theoretical aspects of elastic and inelastic photon-atom scattering (45)
- 1.3 Phillip Platzman      Phenomenology of scattering processes including magnetic and inelastic scattering (45)

Session 2. "Theory: Capabilities and Prospects," Wednesday morning, 8:30 a.m.

Chair: Mihai Gavrilă, FOM Institute, Amsterdam

- 2.1 Dale Koelling      Band calculations and generalizations and what one can learn from them (25)
- 2.2 David Liberman      What is wrong with the Cromer-Liberman anomalous scattering factors and how to improve them (25)
- 2.3 Lynn Kissel      Rayleigh scattering; numerical calculation of theoretical cross sections (25)
- 2.4 Gary Doolen      Anomalous scattering using the local density approximation (15)
- 2.5 David Smith      Sum rule constraints on x-ray data (15)
- 2.6 Edison Liang      NLTE physics issues in scattering at high intensity (15)
- 2.7 Balazs Rozsnyai      Compton scattering in relativistic plasmas (15)
- 2.8 Richard More      Computational model for x-ray scattering in partially ionized plasmas (15)
- 2.9 Frank Biggs      Representations for use of photon cross sections in applications codes (15)
- 2.10 John Rehr      Multiple scattering theory of EXAFS (15)

\*The times in parentheses included the discussion generated by the talk. Although not shown, there was a 20-minute coffee break midway through the sessions.

Session 3. "Basic Experiment," Wednesday evening, 7:30 p.m.

Chair: David Templeton, Lawrence Berkeley Laboratory

- 3.1 Michael Hart X-ray interferometry and synchrotron radiation (20)
- 3.2 Ulrich Bonse X-ray interferometry for measuring x-ray scattering amplitudes (20)
- 3.3 Dudley Creagh Experimental techniques for the measurement of x-ray scattering cross sections and anomalous dispersion corrections (20)
- 3.4 Roman Tatchyn Transmission diffraction interferometry, a novel technique for measuring optical constants (20)
- 3.5 David Templeton Polarization effects of anomalous x-ray scattering (20)
- 3.6 Suhas Ketkar Accurate measurements of incoherent x-ray scattering factors and electron correlations (20)
- 3.7 Jerry Gaines Scattering of x-rays from low-Z materials (20)
- 3.8 Malcomb Cooper Compton scattering and electron momentum determination (20)
- 3.9 Martin Schumacher Rayleigh, Raman, Compton scattering in the 10 to 100 keV energy range (20)

Session 4. "What Lies Ahead," Thursday morning, 8:30 a.m.

Chair: David Attwood, Lawrence Berkeley Laboratory

- 4.1 Kwang-Je Kim Tunable coherent x-rays of arbitrary polarization with next generation storage ring facilities (35)
- 4.2 Bernd Crasemann Studies of atomic processes with future synchrotron radiation facilities (35)
- 4.3 George Brown Novel scattering and absorption spectroscopies with the next generation of synchrotron radiation sources (35)
- 4.4 Dennis Matthews Soft x-ray lasers, demonstration and future plans (35)
- 4.5 Eugene Ice Experimental x-ray scattering cross sections for H<sub>2</sub> and rare atomic gases (20)
- 4.6 Richard Blake Techniques for scattering measurements at Los Alamos and future plans (20)

Session 5. "Applications," Thursday evening, 7:30 p.m.

Chair: Paul Fuoss, AT&T Bell Laboratories

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|----------------------|--|
| 5.1 Brian Stephenson | Time-resolved x-ray scattering (30)  |
| 5.2 Jakob Bohr       | A synchrotron x-ray magnetic scattering study of Holmium (30)  |
| 5.3 Sean Brennen     | Surface x-ray scattering studies (30)  |
| 5.4 Jerome Hastings  | Inelastic x-ray scattering, Mossbauer and back-scattering methods (30)   |
| 5.5 Carl Ludwig      | An x-ray anomalous scattering study of liquid $\text{GeBr}_4$ (20)   |
| 5.6 Jeffrey Hoyt     | Determination of partial structure functions in Al-Ag-Zn alloys by small angle x-ray anomalous scattering (20) |

Session 6A. "X-Ray Optical Techniques," Friday morning, 8:30 a.m.

Chair: John (Hal) Mallett, Lawrence Livermore National Laboratory

- |                        |   |
|------------------------|---|
| 6A.1 Burton Henke      | The application of atomic scattering factors for the characterization of mirrors, multilayers and crystals (20) |
| 6A.2 Jeffrey Kortright | Standing wave scattering techniques using multilayer coatings (20)  |
| 6A.3 Ake Kvick         | X-ray scattering station at the National Synchrotron Light Source (20)  |

Session 6B. "Panel Review of Sessions," Friday morning, 10:10 a.m.

Chair: Nancy Del Grande, Lawrence Livermore National Laboratory

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|-------------------------|--|
| 6B.1 Richard Pratt      | Session 2. Theory: Capabilities and Prospects, reviewed (25)               |
| 6B.2 David Templeton    | Session 3. Basic Experiment, reviewed (25)                                 |
| 6B.3 George Brown       | Session 4. What Lies Ahead, reviewed (25)                                  |
| 6B.4 Paul Fuoss         | Session 5. Applications, reviewed (25)                                     |
| 6B.5 John (Hal) Mallett | Session 6A. X-Ray Optical Techniques, reviewed, and Concluding Remarks (5) |

John (Hal) Mallett, LLNL, "Concluding Remarks"

APPENDIX B

<u>Attendees</u>	<u>Institution</u>
1. Attwood, David	Lawrence Berkeley Laboratory
2. Batterman, Boris	Cornell High Energy Synchrotron Laboratory
3. Biggs, Frank	Sandia National Laboratory, Albuquerque
4. Blake, Richard	Los Alamos National Laboratory
5. Bohr, Jakob	Brookhaven National Laboratory
6. Bonse, Ulrich	Dortmund, West Germany visiting Lawrence Livermore National Laboratory
7. Brennen, Sean	National Bureau of Standards
8. Brown, George	Stanford Synchrotron Radiation Laboratory
9. Cheng, Kwok Tseng	Lawrence Livermore National Laboratory
10. Cooper, Malcomb	University of Warwick, England
11. Crasemann, Bernd	University of Oregon, Eugene
12. Creagh, Dudley	Royal Military College, Duntroon, Australia
13. Del Grande, Nancy	Lawrence Livermore National Laboratory
14. Doolen, Gary	Los Alamos National Laboratory
15. Ebert, Paul	Lawrence Livermore National Laboratory
16. Fuoss, Paul	AT&T Bell Laboratories, Holmdel, NJ
17. Gaines, Jerry	Lawrence Livermore National Laboratory
18. Gavrilu, Mihai	FOM Institute, Amsterdam, visiting University of Pittsburgh
19. Hart, Michael	Schuster Laboratory, Manchester, England
20. Hastings, Jerome	Brookhaven National Laboratory
21. Henke, Burton	Lawrence Berkeley Laboratory
22. Hoyt, Jeffrey	University of California, Berkeley
23. Hubbell, John	National Bureau of Standards
24. Ice, Gene	Oak Ridge National Laboratory
25. Ketkar, Suhas	Indiana University, Bloomington, IN
26. Kim, Kwang-Je	Lawrence Berkeley Laboratory
27. Kissel, Lynn	Sandia National Laboratory, Albuquerque
28. Koelling, Dale	Argonne National Laboratory
29. Kortright, Jeffrey	Lawrence Berkeley Laboratory
30. Kwick, Ake	Brookhaven National Laboratory
31. Liang, Edison	Lawrence Livermore National Laboratory
32. Liberman, David	Lawrence Livermore National Laboratory
33. Ludwig, Carl	Stanford Synchrotron Radiation Laboratory
34. Mallett, John H. (Hal)	Lawrence Livermore National Laboratory
35. Matthews, Dennis	Lawrence Livermore National Laboratory
36. More, Richard	Lawrence Livermore National Laboratory
37. Platzman, Phillip	AT&T Bell Laboratories, Murray Hill, NJ
38. Poppe, Carl	Lawrence Livermore National Laboratory
39. Pratt, Richard	University of Pittsburgh
40. Rehr, John	University of Pittsburgh
41. Rozsnyai, Balazs	Lawrence Livermore National Laboratory
42. Saloman, Ed	National Bureau of Standards
43. Schumacher, Martin	University of Goettingen, West Germany
44. Scofield, James	Lawrence Livermore National Laboratory
45. Smith, David	Argonne National Laboratory
46. Stephenson, Brian	IBM Research Center
47. Tatchyn, Roman	Stanford Synchrotron Radiation Laboratory
48. Templeton, David	Lawrence Berkeley Laboratory
49. Templeton, Liselotte	Lawrence Berkeley Laboratory

50. Thompson, Carol  
51. Tirsell, K. Glenn

University of Houston and IBM Research Center  
Lawrence Livermore National Laboratory