MASTER

LOW-ENERGY X-RAY AND ELECTRON PHYSICS AND
APPLICATIONS TO DIAGNOSTICS DEVELOPMENT
FOR LASER-PRODUCED PLASMA RESEARCH

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This final report describes a collaborative extension of an on-going research program in low-energy x-ray and electron physics into particular areas of immediate need for the diagnostics of plasmas as involved in laser-produced fusion research. It has been for the continued support for one year of a post-doctoral research associate and for three student research assistants who have been applied to the following specific efforts:

1. The continuation of our research on the absolute characterization of x-ray photocathode systems for the 0.1 to 10 keV photon energy region. The research results were applied collaboratively to the design, construction and calibration of photocathodes for time-resolved detection with the XRD and the streak and framing cameras.
2. The design, construction and absolute calibration of optimized, "bolt-on" spectrographs for the absolute measurement of laser-produced plasma spectra. These have about 1 eV resolution and selectable, parallel spectral channels in several bands of the 0.1 to 1.0 keV region.
3. The calculation and tabulation of atomic scattering factors for the 100 to 2000 eV photon energy region which include the important effects of anomalous dispersion. These have been applied immediately to (a) the tabulation of refractive indices of materials that are appropriate for total-reflection mirror monochromator systems and for improved and detailed characterization of their reflection versus angle and photon energy characteristics; (b) the determination of the percent and integrated reflectivities and the resolution of crystals and multilayers (molecular, sputtered and evaporated) that are appropriate for laser-produced plasma spectroscopy; and (c) the calculation of the diffuse scattered intensity from material surfaces that may constitute significant background radiations in high intensity plasma studies.

The results on our studies on x-ray photocathodes are presented here in the recently published report, "The Characterization of X-Ray Photocathodes in the 0.1-10 keV Photon Energy Region," J. Appl. Phys. 52, 1509 (1981), by B. L. Henke, J. P. Knauer and K. Premaratne.

The work on the development of quantitative x-ray spectroscopy for low-energy x-ray diagnostics has been reviewed by this principal investigator and preprints are attached here of reports that have been presented at the 1981 APS Topical Conference on Low Energy X-Ray Diagnostics, Monterey, June 1981:

- (a) "Low Energy X-Ray Spectroscopy with Crystals and Multilayers," Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics (November 1981), B. L. Henke.
- (b) "A Sensitometric Calibration of the RAR 2497 Film for the Low Energy X-Ray Region," Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics (November 1981), E. R. Dietz, T. S. Durland, B. L. Henke and M. A. Tester.

Finally, a description of our work on the atomic scattering factor description of low-energy x-ray interactions has also been presented at the Monterey Conference and preprints are attached here:

- (a) "Low Energy X-Ray Interactions: Photoionization, Scattering, Specular and Bragg Reflection," Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics (November 1981), B. L. Henke.
- (b) "Appendix: The Atomic Scattering Factor, $f_1 + if_2$, for 94 Elements and for the 100 to 2000 eV Photon Energy Region," Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics (November 1981).

As general background description of this on-going program in low-energy x-ray and electron physics, we have appended:

1. Research Publications (Published or In Press) 1977-1981;
2. Research Papers Presented at Scientific Meetings by this Principal Investigator, 1977-1981;
3. First-Page Abstracts of Research Publications, 1977-1981.

The characterization of x-ray photocathodes in the 0.1–10-keV photon energy region

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A method and an instrument are described for the measurement of the absolute quantum yield for front-surface and transmission photocathodes in the 0.1–10-keV photon energy region. The total and the secondary electron photoemission yields have been measured for the Al, Au, CuI, and CsI photocathodes as required for the absolute calibration of the x-ray diode detectors and for the x-ray streak cameras. The relative secondary electron yields have also been measured for the same photocathodes by high resolution electron spectroscopy of the secondary electron energy distributions, which are in good agreement with the absolute yield measurements. The secondary electron yield of CsI is ten to one-hundred times higher than that for Au in the 0.1–10-keV region and with a secondary energy distribution that is appreciably sharper. For these reasons, CsI should be an effective photocathode for sensitive, time-resolved spectroscopy into the picosecond region. It is verified experimentally that the secondary electron quantum yield varies approximately as $E\mu(E)$, with E as the photon energy and $\mu(E)$ as the photoionization cross section, and that the primary (fast) electron quantum yield is a small fraction of the total yield and varies approximately as $E^2\mu(E)$. A simple model for x-ray photoemission is described which leads to semiempirical equations for front- and back-surface secondary electron photoemission as based upon an escape depth parameter that may be obtained from yield-versus-photocathode thickness data. The model predictions are in good agreement with experiment.

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I. INTRODUCTION

Time-resolved x-ray spectroscopy has become of considerable importance in the temperature density composition diagnostics of high-temperature plasmas involved in controlled thermonuclear fusion studies which utilize laser, particle beam, or magnetic compression-confinement production. The time duration of the associated x-ray emission ranges from picoseconds to seconds. Time-resolved x-ray spectroscopy is also important in the development of super-radiant, pulsed x-ray sources, their application to studies of the radiation effects of x-ray bursts upon materials, and the x-ray analysis of atomic, molecular, and solid-state time-resolved processes into the picosecond region.

The electron currents that are emitted by photocathodes under x-ray excitation can be a very effective basis for time resolved spectroscopic measurement using x-ray diode or streak camera detection.^{1–5} In the latter, an x-ray spectrum can be established along a slit-defined transmission photocathode of the streak camera by using focussing filter-total-reflection monochromator, crystal/multilayer arrays, or nonfocussing, Bragg reflecting crystal/multilayer analyzer systems.

In time-resolved x-ray spectroscopy, the ultimate limit on the achievable time resolution is the quantum conversion efficiency of the photocathode (which determines signal statistics) and the energy spread of the emitted electrons as is noted in Fig. 1 (which determines the time resolution).⁶ The relatively small fraction of fast electrons that is photoemitted is effectively blocked by the electron optical apertures of

the typical streak camera. In Fig. 2 the difference in the arrival time at the output end of the streak camera is given as a function of the energy width Δ of the secondary electron energy distribution, the extraction field ϵ_0 , and of the geometry of the camera. In addition to the absolute yield-versus-photon energy and the shape of the secondary electron distribution curves, other important characteristics of the x-ray photocathode are its stability, reproducibility, simplicity of spectral response, and the linearity of its time response. Described here is a method and an instrument for the measurement of the absolute total and secondary electron yields

FIG. 1. In the 0.1–10-keV photon energy region the larger fraction of the electrons that are emitted are the secondary electrons, typically as a narrow distribution below 10 eV. The higher energy, fast electron photoemission consists of relatively sharp elastically scattered photoelectrons and Auger electron "lines" along with a much larger number of inelastically scattered electrons in their low-energy tail region.

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TEMPORAL RESOLUTION LIMIT, τ

$$\tau = 3.37 \frac{(\Delta)^{1/2}}{e_0} \left\{ 1 + \frac{1}{4} \left(\frac{L}{S} - 2 \right) \left(\frac{\Delta}{eV_0} \right)^{1/2} \dots \right\} \text{ PICOSECONDS}$$

Δ = SECONDARY ELECTRON ENERGY SPREAD IN eV

e_0 = EXTRACTION FIELD, V_0/S IN KV/MM

FIG. 2. Schematic of an x-ray streak camera for time-resolved x-ray spectroscopy. Its ultimate time resolution is determined by the difference in arrival time τ at the output end of the camera associated with the energy width Δ of the secondary electron distribution emitted from the transmission photocathode. For a secondary electron energy spread Δ of 2 eV and an extraction field e_0 of 5 kV/mm, the time resolution τ is approximately 1 ps. (The fast electron photoemission is essentially blocked electron optically in the streak camera.)

(electrons emitted per normally incident photon) for both front-surface and transmission photocathodes in the 0.1–10-keV photon energy region and the application to the characterization of photocathode materials of current practical importance such as gold and cesium iodide. In addition to the measurements of the total electron emission in the secondary and primary electron components, high-resolution electron spectroscopic measurements of the secondary electron energy distributions for these photocathodes are also presented. A simple model for the quantum yield of x-ray photoemission is outlined here that includes the effect of photocathode thickness upon the front- and back-surface emissions.

II. THE MEASUREMENT OF X-RAY PHOTOEMISSION

The facility that has been developed for making absolute yield measurements in the photon energy region of 0.1–10 keV is shown in Fig. 3. Six filtered fluorescent sources of essentially monochromatic characteristic x radiations may be excited by a closely coupled, 2–4 kW demountable x-ray source of strong characteristic line radiation of photon energy just above that of the fluorescent line being used.⁷ The photocathodes are also brought in as closely as possible to the fluorescent source in order to maximize the photoemission currents to be measured. The absolute x-ray flux per steradian at the same take-off angle from a 3-cm fluorescent source disk is measured by a calibrated flow proportional counter at the end of an extended vacuum path and with an accurately defined pinhole aperture (to limit the counting rates to less than ~ 5000 c/s for negligible coincidence loss).

An eight-position, front-surface photocathode Teflon sample holder (four positions for transmission photocath-

odes) has been accommodated in order to allow precise relative measurement, for example, of a series of different photocathode materials, or of different photocathode thicknesses.

A cylindrical "grid" technique has been developed for the retarding of the secondary electron emission current in the determination of the primary or fast electron components. This cylindrical grid system is so designed that no direct x-radiation can reach surfaces that can contribute background emission currents which might return to the photocathode when it is at a relatively positive, retarding potential. High transparency mesh surfaces are placed in front of surfaces which are at appreciably higher positive potential, thereby trapping the large angle photoemitted electrons which might otherwise excite secondary electron background. This cylindrical grid method for separating the secondary from the total photoemission current is illustrated as applied to both front-surface and transmission photocathode characterizations in Figs. 4, 5, 6, and 7. As illustrated here, detailed equipotential maps of the accelerating and retarding fields have been compared along with photoemitted electron ray traces⁸ in order to determine the potential "hill" characteristics of the cylindrical grids.

The filter-window material on the proportional counter aperture is identical to that on the entrance aperture to the photocathode section so that their transmissions cancel in the absolute yield measurements. By using a similar material on the back, substrate surface of the transmission photocathodes, the back-surface photoemission current is effectively cancelled by that from the adjacent entrance window surface (0.8-cm separation) thereby improving the measurement statistics in the difference measurements.

FIG. 3. Instrument for the relative and absolute measurement of the quantum yields for front-surface and transmission photocathodes in the 0.1–10-keV photon energy region. Characteristic fluorescent line sources are excited by a closely coupled x-ray source of strong line radiation of photon energy just above that of the fluorescent lines. The fluorescent line intensities are measured by a calibrated proportional counter which views the source at the same take-off angle as does the photocathode. The filter material between the source and the photocathode is identical to that on the proportional counter aperture. The monochromaticity of the fluorescent sources under similar excitation and filtering are evaluated spectroscopically and are monitored by a multichannel pulse height analyzer during the measurements. The electrometer current output is converted proportionally to a frequency from 0 to 25 kHz for rapid and precise digital signal averaging.

FIG. 4. Cylindrical grid geometry for front-surface photoemission measurement. Illustrating the retarding field, potential hill characteristics and electron ray traces for the measurement of the fast electron photoemission component.

The x-radiation that passes through the side-window proportional counter is limited by the entrance pinhole window to a narrow beam that just misses the central anode wire and, if not absorbed, proceeds through an exit hole in the opposite side and into a positive potential electron trap region. The effective absorption path between the two apertures is 3.51 cm. The anode wire diameter is $50\ \mu$. When possible, the photon absorption efficiency is set between 85

and 95% for a given photon energy by the choice of the counter gas and its pressure. This "pressure tuning" minimizes ionization charge loss at the entrance window and photon loss through the exit aperture and provides minimum-width pulse height distributions.⁷ A multichannel pulse height analyzer is used to monitor the output pulses of the proportional counter in order to verify that a given fluorescent line source is optimally excited and filtered for

FIG. 5. Total yield measurement of front-surface photoemission.

FIG. 6. Cylindrical grid geometry for back surface photoemission measurement. Illustrating the retarding field, potential hill characteristics and electron ray traces for the measurement of the fast electron photoemission component.

minimum background x-radiation.

In Table I are presented a list of the fluorescent line sources that were employed in the measurements that are reported here along with a description of the excitation, filtering, and flow proportional counter parameters that were chosen to obtain the calibrated photon excitation to the photocathodes.

The photocathode materials were vacuum evaporated upon chromium-coated microscope slide substrates and were mounted upon a rotatable, insulating Teflon structure. The vibrating reed preamplifier head of a Carey 401 Electrometer was connected through a rigid coaxial section to a low-loss feedthrough and to a spring contact upon a polished button which fastens each photocathode to the holder. Typi-

cal measurement current levels for these studies were between 10^{-12} and 10^{-15} A. A mechanical shutter for the x-ray beam was provided between the source and the photocathode to permit a determination of the effective background current ($\sim 10^{-17}$ A).

For rapid and convenient signal averaging, the electrometer output current was converted by a variable frequency oscillator circuit (IC-Raytheon 4151) to a frequency that is precisely proportional to the current and in the 0-25-kHz region. The quantum yield (as the charge collected per photon incident upon the photocathode) is measured by counting the number of cycles within a time interval that is determined by that required to collect a set number of photons at the proportional counter (typically 10 000 counts).

FIG. 7. Total yield measurement of back-surface photoemission.

TABLE I. Parameters for the calibrated fluorescent line excitation sources.

λ (Å)	E (eV)	Fluorescent source	Exciting source	Filter	Filter thickness	Filter transmission (%)	Proportional counter		
							Gas	Pressure	Efficiency (%)
1.79	7469	Ni-K α	Cu-K	Ni	12 μ	47	P-10	760	53
1.94	6397	Fe-K α	Cu-K	Ni	12 μ	38	P-10	760	69
2.29	5411	Cr-K α	Cu-K	Ni	12 μ	20	P-10	760	84
4.16	2981	Ag-L α	Cr-K	Ag	0.5 μ	77	P-10	760	85
5.41	2292	Mo-L α	Cr-K	Ag	0.5 μ	59	P-10	760	85
7.13	1739	Si-K α	Cr-K	Ag	0.5 μ	35	P-10	760	98
8.34	1486	Al-K α	Cr-K	Ag	0.5 μ	22	P-10	760	100
9.89	1254	Mg-K α	Al-K	Mg	6.6 μ	57	Propane	200	80
13.3	930	Cu-L α	Al-K	Mg	6.6 μ	28	Propane	200	98
14.6	852	Ni-L α	Al-K	Mg	6.6 μ	20	Propane	200	99
17.6	705	Fe-L α	Ni-L	Fe	0.6 μ	36	Propane	75	95
18.3	677	F-K α	Ni-L	Fe	0.6 μ	33	Propane	75	96
23.6	525	O-K α	Ni-L	Formvar	52 $\mu\text{g}/\text{cm}^2$	66	Propane	50	99
31.6	392	N-K α	Cu-L, O-K*	Formvar	52 $\mu\text{g}/\text{cm}^2$	43	Propane	50	100
44.7	277	C-K α	Cu-L, O-K*	Formvar	52 $\mu\text{g}/\text{cm}^2$	84	Propane	100	82
64.4	193	Mo-M ζ	C-K	Formvar	52 $\mu\text{g}/\text{cm}^2$	65	Propane	50	88
82.1	151	Zr-M ζ	C-K	Formvar	52 $\mu\text{g}/\text{cm}^2$	46	Propane	50	98
114	109	Be-K α	C-K	Formvar	52 $\mu\text{g}/\text{cm}^2$	20	Propane	50	100

*Oxidized copper anode.

III. EXPERIMENTAL RESULTS

A. Front-surface photoemission—thick photocathodes

For x-ray diode detectors, effective front-surface emission photocathodes have been aluminum, gold, the semiconductor copper iodide, and the insulator cesium iodide. These have been included in this study. The materials, vacuum evaporated as thick photocathode systems upon chromium-coated microscope slide substrates, were handled in a dry-nitrogen atmosphere outside the vacuum systems. The total yields and the fast, primary electron yields (secondary electrons retarded by a -50 -V potential "hill") were measured for eighteen photon energies in the 0.1 - to 10 -keV region. The total yield data are presented in Figs. 8, 9, 10, and 11. In Fig. 12 are presented the associated curves for the measured ratios of the primary yield (fast electron component) to the total yield, Y_p/Y_T . From these data it may be noted that the dominant photoemission current is that of the secondary electrons, and that for the several photocathodes characterized here, the primary yield are very similar and the insulator and semiconductor photocathodes, CsI and CuI, have considerably higher secondary electron yields than do the metal photocathodes Al and Au.

It is of interest to compare here the secondary electron energy distributions for these same photocathodes. To measure these, the photocathodes were transferred to an electron spectrograph and analyzed with at about 0.01 -eV resolution as has been described previously.^{9,10} Presented in Figs. 13 and 14 are spectra for the four photocathodes as photoexcited by C-K α (227 eV) and Cu-K α (8080 eV). The peak intensities of the distributions are given relative to that for the gold photocathode. Also noted here are the peak positions E_{KP} and the full width at half maximum Δ for each secondary electron energy distribution.

It is important to note that, as is illustrated here, there is no significant change in the shape of the secondary electron energy distributions for a given photocathode in the 0.1 - to 10 -keV excitation region. It is also of considerable practical importance that the CuI and CsI photocathodes do have the narrow secondary electron energy distributions and high quantum efficiency that is required for sensitive time-resolved spectroscopy in the picosecond range¹¹ (see Fig. 2).

By measuring the area under the secondary electron energy distribution curves, as those presented in Figs. 13 and 14, we have obtained the relative secondary electron yields for photocathodes as excited and analyzed under identical conditions. In Table II are presented the secondary electron

FIG. 8. Front-surface, total quantum yield for a $1400\text{-}\text{\AA}$ evaporated aluminum photocathode. [Compared to $E_{\mu}(E)$ for Al_2O_3 .]

FIG. 9. Front-surface total quantum yield for a 300-Å evaporated gold photocathode. [Compared to $E\mu(E)$ for Au.]

FIG. 11. Front-surface total quantum yield for a 3000-Å evaporated cesium iodide photocathode. [Compared to $E\mu(E)$ for CsI.]

yield of cesium iodide relative to that for gold as determined by the total-and-retarded absolute yield measurements described above and by the electron spectroscopy¹⁰ of the secondary distributions. As shown here, the agreement between these independent methods is very good.

In order to define an appropriate thickness for the "thick", front-surface photocathodes and to measure the effective escape depth of the secondary electron emission for a given photocathode, the secondary electron yields have been measured as a function of film thicknesses. An example of these determinations is presented in the yield-versus-thickness data of Fig. 15 for the cesium iodide photocathode. (A chromium substrate was used for CsI films because its very low photoemission yield relative to that for CsI allows only a negligible contribution to the measured yields.) The film thicknesses greater than a few hundred angstroms were measured by multiple-beam interferometry; smaller thicknesses were determined by extrapolation using the thickness depen-

dence upon an inverse square of the distance of the sample from an effective point evaporation source. These data suggested our use of 3000-Å CsI films for the thick photocathode measurements that are described here and which would be appropriate for x-ray diode detector applications.

FIG. 10. Front-surface total quantum yield for a 1100-Å evaporated copper iodide photocathode. [Compared to $E\mu(E)$ for CuI.]

FIG. 12. Ratio of the primary (fast) electron yield to the total electron yield for Au, Al, CuI, and CsI. According to the x-ray photoemission model presented here and based upon an effective escape depth for the primary electron photoemission that is proportional to the range given by the Bethe-Bloch continuous-slowing-down-approximation, the ratio Y_P/Y_T is predicted to vary as $E^{-0.88}$ for these photocathodes.

TABLE II. $Y_s(\text{CsI})/Y_s(\text{Au})$ for thick photocathode secondary electron yields. Relative Yields— $Y_s(\text{CsI})/Y_s(\text{Au})$.

Photon energy (eV)	From absolute yield	From secondary electron energy distributions
277	11	10
1487	44	42
8080	34	34

B. Back-surface photoemission—transmission photocathodes

Gold and cesium iodide transmission photocathodes are currently being applied in x-ray streak cameras for time-resolved spectroscopy into the picosecond range.¹¹ We have presented the back-surface secondary electron emission yield-versus-photon energy data for the 0.1–10-keV region for these photocathodes in Figs. 16 and 17. The transmission photocathode films were of about 250- and 1000-Å thickness, respectively, and were vacuum evaporated upon carbon foil substrates of about 50 μg per cm^2 mass thickness. The x-ray transmissions of the substrate carbon foils were measured and these values were used to obtain the secondary electron yield per normally incident photon as transmitted to the front surface of the photocathode film. Carbon foil substrates were chosen because these have good mechanical strength, low attenuation for the low-energy x-rays, and are conducting. Because of the very low photoemission efficiency of the carbon substrates, it is expected that these yield data are essentially independent of the substrate contribution and would be the same for the equivalent self-supporting film system.

In Figs. 18 and 19 are presented the back-surface yield-versus-photocathode film thickness for the gold and cesium iodide systems. Because of the very broad maxima charac-

teristic of the yield-versus-thickness curves for the transmission photocathodes, we have chosen the thicknesses of 250 and 1000 Å as appropriate for the Au and CsI transmission photocathodes, which allow somewhat greater uniformity and strength without a serious decrease in yield from an optimum value for the low-energy x-rays.

IV. A SIMPLE MODEL FOR FRONT- AND BACK-SURFACE X-RAY PHOTOEMISSION YIELDS AND FOR THE EFFECT OF PHOTOCATHODE THICKNESS: COMPARISON WITH EXPERIMENTAL RESULTS

In a previous work¹⁰ we presented a detailed phenomenological model for x-ray photoemission for thick photocathodes. Here we extend this description to include the effect of photocathode thickness for the thin metal or insulator photocathode for which both front- and back-surface photoemission are excited by incident x radiation.

We had noted that the x-radiation energy that is deposited within the photocathode is converted through photoelectric absorption to that of photoelectrons and subsequently to emitted Auger electrons and fluorescent radiation. Nearly all of this deposited energy is transformed to that of primary electrons within the photocathode except for a small fraction that is associated with the primaries and fluorescence that escapes through the photocathode surface. The energy of these internal primaries is initially and completely transformed to the excitation energy of secondary electrons (mostly by promoting valence-band electrons to the conduction band and by the deexcitation of excited plasmons). Heuristically we can relate the number of secondaries N that are excited within a unit photocathode area of effective escape depth λ_s in a thick photocathode to the x-radiation energy deposited by the expression

$$N\bar{E}_{KS} \approx I_0 \rho E \mu(E) \lambda_s, \quad (1)$$

where $\bar{E}_{KS}$ is the mean energy of the excited secondaries, I_0 is the number of photons per unit area normally incident and

FIG. 13. Secondary electron energy distributions for Au, Al, CuI, and CsI photocathodes (as measured in Figs. 8–11). Excited by C-K α (277 eV) x radiation.

FIG. 14. Secondary electron energy distributions of Au, Al, CuI, and CsI photocathodes (as measured in Figs. 8-11). Excited by Cu-K α (8080 eV) x radiation. Note that the shapes of these distribution curves are essentially the same as those excited by the C-K α (277 eV) x radiation.

of energy E , $\mu(E)$ is the mass photoionization cross section, and ρ is the mass density. Assuming that the number of secondaries emitted per incident photon (the yield, Y_s for a thick photocathode) is simply proportional to that number of internally excited secondaries within the escape volume, we may then predict that

$$Y_s \sim \rho E \mu(E) \lambda_s / \bar{E}_{KS}. \quad (2)$$

We have not been able to detect any significant change in the energy distribution of the emitted secondary electrons with photon energy in the 0.1-10-keV region as is illustrated here in Figs. 13 and 14. This implies that the internal energy distributions are also independent of the x-ray photon energy and that $\bar{E}_{KS}$ is a constant for a given photocathode material. We may therefore predict for the yield of secondary electrons from a thick photocathode the relation

$$Y_s = K_s \rho E \mu(E) \lambda_s. \quad (3)$$

Applying the same reasoning for the emission of the primary electrons, we note that $\bar{E}_{KP}$ for the internal distribution of primaries would be essentially proportional to the incident photon energy E , and we obtain from a relation analogous to Eq. (2),

$$Y_p = K_p \rho \mu(E) \lambda_p. \quad (4)$$

Because λ_s , the escape length, for secondaries is independent of the photon energy, the secondary electron yield dependence upon the x-ray photon E should be approximately as $E \mu(E)$. This is confirmed by a comparison of the $E \mu(E)$ curves that are presented along with the log-log plots of the experimental yield data in Figs. 8-11. (The total yield plotted in these figures is mostly that of secondary electron emission.)

An escape depth for the primaries which are emitted into the sharp, elastically scattered photoelectron and Auger electron lines (as depicted in Fig. 1) may be a mean free path, and, for the kilovolt region, may depend upon the energy^{9,12,13} as approximately $E_K^{0.8}$. However the total primary

yield that is measured here, Y_p , is mostly that of the fast electrons which have suffered many inelastic collisions before escaping (into the low-energy tails of the line spectra as illustrated in Fig. 1) and for these, the effective escape depth λ_p is more accurately described as a practical range. Its energy dependence, therefore, might be obtained for the kilovolt region by a logarithmic extrapolation of the Bethe-Bloch continuous-slowing-down-approximation range given in the tables of Pages et al. as approximately the relation λ_p (CSPA) $\approx R_0 E_K^{1.9}$.^{14,15} We may thus predict then since the primary energies should increase as the photon energy, the primary yield Y_p depends upon photon energy as approximately $E^{1.9} \mu(E)$. It then follows from Eqs. (3) and (4) that the ratio Y_p/Y_s should depend upon the x-ray photon energy in the kilovolt region as approximately $E^{0.9}$. This dependence is suggested by the experimental data for Y_p/Y_s presented in Fig. 12 ($Y_p/Y_s = Y_p/(Y_s + Y_p) \approx Y_p/Y_s$, for $Y_p \ll Y_s$).

FIG. 15. Front-surface secondary electron yield for CsI vs photocathode film thickness and t according to a yield equation predicted by the x-ray photoemission model presented here. (The CsI was evaporated upon a chromium substrate of relatively very low photoemission efficiency.)

In the detailed analysis of secondary electron photoemission that is presented in Ref. 10 are predicted this photon energy dependence through the factor $E\mu(E)$ and also the secondary electron energy distributions for photoemission from metals, semiconductors, and insulators for thick photocathodes. As in Kane's secondary electron transport model,¹⁶ we have assumed in this analysis that an electron-electron collision will drop the energy of a random-walking secondary electron to below the vacuum level and hence eliminate it from the group of electrons that may escape from the photocathode surface. Following Kane's notation, we define the linear scattering cross section (inverse mean free path) for electron-electron collisions as b . The electron-phonon collision cross section is defined as a for which the associated energy loss per collision is very small. For a given photocathode, a and b are assumed to be constants. In Ref. 10, we have used Kane's transport model to predict an isotropic distribution of secondaries just inside the photocathode surface and have then applied the usual escape cone integral over all the secondary energies to determine the secondary electron energy distribution and yield as emitted from the photocathode surface. In this model we neglected any enhancement of the secondary emission resulting from a reflection of those secondaries that are outside the escape cone (into the photocathode and possibly "wandering" back by a random walk to the surface and escaping). For metals, any reflecting secondaries would most likely suffer an electron-electron collision ($b \gg a$) in order to return and would thereby be dropped to below the vacuum level. For insulators, for which electron-electron collisions are unlikely ($b \ll a$), it is suggested in Ref. 10 that the internal reflection of secondaries may contribute to a small enhancement of photoemission. This enhancement factor, however, is independent of photon energy and thus is essentially constant for a given photocathode.

As outlined in the Appendix, we have applied a similar analysis for the case of thin photocathodes for which both front- and back-surface photoemission is involved as illustrated in Fig. 20. We have simply placed a limit of t for the

FIG. 16. Back-surface secondary electron quantum yield for a 230-Å Au transmission photocathode.

FIG. 17. Back-surface secondary electron quantum yield for a 1020-Å CsI transmission photocathode.

thickness of the photocathode instead of infinity as in Kane's original analysis for a semi-infinite photocathode and as has been done by Pong et al.¹⁷ for a finite photocathode. We neglect any contributions to the yield from the front- or back-surface reflections because it can be shown that such are significant only if the photocathode thickness approaches a value equal to the escape length l_s . As will be shown in the following, a practical thickness for the x-ray photocathode will be several times greater than this escape length value. In addition to our considering enhancement of emission resulting from internal reflections to be small and constant, we have also considered the mean attenuation length for the photons within the photocathode, $(\mu p)^{-1}$, to be very large as compared with the mean free paths b^{-1} and a^{-1} .

This simple extension of our x-ray photoemission model results in the following relations for the secondary electron emission yields for the front and back surfaces Y_f and Y_b as a function of the photocathode thickness t : front surface,

$$Y_f = KpE\mu(E) \left(\frac{c}{u(u+c)} \right) \left(\frac{1-e^{-ut}}{1+\delta e^{-ut}} \right), \quad (5)$$

FIG. 18. Back-surface secondary electron yield for Au vs. transmission photocathode film thickness and fit according to a yield equation predicted by the x-ray photoemission model presented here.

back surface,

$$Y_b = K\rho E\mu(E) \left(\frac{ce^{-\mu x}}{u(u+c)} \right) \left(\frac{1-e^{-\mu t}}{1+\delta e^{-\mu t}} \right). \quad (6)$$

Here, as functions of the linear cross sections for electron-phonon and electron-electron scattering, a and b , we have introduced the parameters:

$$c = (a + b)$$

$$u = (c^2 - ac)^{1/2} = (b^2 + ab)^{1/2},$$

$$\delta = (c - u)/(c + u).$$

K is a material constant which depends upon the electronic constants of the photocathode material as the band-gap energy E_G and the electron affinity E_A for insulators, and upon the Fermi energy E_F and the work function W for metals (as discussed in Ref. 10).

As shown in Kane's one-dimensional random-walk analysis for secondary electron transport to the surface, u^{-1} is the escape length for a photocathode of infinite thickness and defined here as an average escape length, λ_s , measured normal to the surface. (The mean free paths for electron-phonon and electron-electron scattering, a^{-1} and b^{-1} , as adopted here from Kane's one-dimensional random-walk analysis, are the averages of the projections along the direction normal to the photocathode surface of the actual three-dimensional random-walk scattering path segments. These one-dimensional mean free paths have been shown by exact three dimensional random-walk analyses to be approximately one-half the magnitude of the corresponding actual mean free paths.¹⁰)

For insulators, $b \ll a$, and therefore $u \approx (ab)^{-1/2}$ and $\delta \approx 1$. Defining an escape length λ_s as equal to $(ab)^{-1/2}$ for insulators, we obtain from Eqs. (5) and (6)

$$Y_f = K\rho E\mu(E)\lambda_s \tanh(t/2\lambda_s) \quad (7)$$

and

$$Y_b = K\rho E\mu(E) e^{-\mu t/2\lambda_s} \tanh(t/2\lambda_s). \quad (8)$$

For metals, $b \gg a$, and therefore $c \approx b$, $u \approx b$, and $\delta \approx 0$. Defining an escape length λ_s for metals to be equal to b^{-1} , we may obtain from Eqs. (5) and (6)

FIG. 20 Front- and back-surface emission geometry for the transmission photocathode.

$$Y_f = K\rho E\mu(E)\lambda_s(1 - e^{-t/\lambda_s}) \quad (9)$$

and

$$Y_b = K\rho E\mu(E)\lambda_s e^{-t/\lambda_s}(1 - e^{-t/\lambda_s}). \quad (10)$$

Here λ_s is the x-ray attenuation length, $(\mu\rho)^{-1}$.

In Fig. 15 is shown a fit of Eq. (7) to the experimental data of yield-versus-thickness for the insulator, cesium iodide on a chromium-coated substrate. Because the trend of the experimental data is to pass through the origin and because the yield at 277 eV for chromium is very small as compared with that of CsI (about 3%), it is suggested that the substrate contributes a relatively small effect upon these yield data. The best fit parameter λ_s , equal to 250 Å, is in good agreement with the measurements of the escape length for secondary electrons emitted from CsI crystals and films by Iyengar et al.¹⁰ of 215 Å.

By maximizing the transmission photocathode yield Y_t as given in Eqs. (8) and (10), we obtain the following expressions for the optimum thickness of insulator and metal photocathodes:

$$t_{\text{opt}} = \lambda_s \sinh^{-1}(\lambda_s/\lambda_s), \quad (11)$$

for metals,

$$t_{\text{opt}} = \lambda_s \ln(\lambda_s/\lambda_s). \quad (12)$$

For the insulator, cesium iodide (choosing λ_s equal to 250 Å with photon energies of 193, 525, and 2292 eV, the x-ray attenuation lengths are 3620, 5790, and 13 470 Å, respectively, and the corresponding values for the optimum thicknesses are 840, 940, and 1170 Å, respectively. For the gold photocathode (choosing λ_s equal to 40 Å^{10,20}) with the same photon energies of 193, 525, and 2292 eV, the x-ray attenuation lengths are 397, 440, and 1409 Å, respectively, and the corresponding values for the optimum thicknesses are 92, 96, and 142 Å, respectively. These values are well within the experimental precision limits suggested for the optimum thicknesses by the data presented in Figs. 18 and 19 to which we have fit the predicted Y_b vs t relations given in Eqs. (7) and (10).

V. CONCLUSIONS

The secondary electron quantum yield varies with the

FIG. 19 Back-surface secondary electron yield for CsI on transmission photocathode thickness and fit according to a yield equation predicted by the x-ray photoemission model presented here.

photon energy approximately as $E\mu(E)$ has been demonstrated here for the metals, gold, and aluminum, for the semiconductor, copper iodide, and for the insulator, cesium iodide. The primary electron yield varies less rapidly with photon energy and approximately as $E\mu^2(E)$. [$\mu(E)E^n$ with n typically between 2.5 and 3.]

The secondary electron yield for CsI is ten to one-hundred times higher than that for Au in the 0.1–10-keV region. This increased efficiency may be attributed in part to its larger escape depth (250 Å as compared to 40 Å) and to its low electron affinity. Its high quantum yield and relatively narrow secondary electron energy distribution suggest that CsI would be a very effective photocathode for sensitive time-resolved x-ray spectroscopy into the picosecond region.

A simple model for x-ray photoemission has been extended to include the effect of photocathode thickness, which does predict the photon energy dependence for the secondary and the primary electron quantum yields and the dependence of front- and back-surface secondary electron yield upon photocathode thickness. Relatively simple expressions have been derived and can be used as semiempirical equations for quantum yield and based upon the parameter, λ_s (the escape length for the corresponding semi-infinite photocathode) which may be determined experimentally from yield-versus-thickness data. The predictions of this phenomenological model are in good agreement with the experimental measurements.

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APPENDIX: SECONDARY ELECTRON EMISSION FROM A FINITE PHOTOCATHODE: ONE-DIMENSIONAL, RANDOM-WALK ANALYSIS

Our derivation of relations (5) and (6) for the front- and back-surface photoemission from a finite x-ray photocathode is based upon a one-dimensional random-walk analysis method of Kane¹⁶ and upon the following assumptions

(1) The number of emitted secondary electrons is proportional to the number that have transported to the emission surface by electron-phonon scattering only. Electron-electron scattering effectively drops the energy of the secondaries below that of the vacuum level.

(2) The number of electrons is negligible that have electron-phonon scattered to the surfaces and then reflect back into the photocathode volume and manage to random walk by electron-phonon scattering to these surfaces and to escape.

(3) The probabilities per unit pathlength normal to the surfaces for electron-phonon and for electron-electron scattering, a and b respectively, are constants [independent of

secondary electron energy].

(4) The mean attenuation length for the x-ray photons, $(\mu\rho)^{-1}$, is very large as compared to the one-dimensional mean free paths, a^{-1} and b^{-1} , for electron-phonon and electron-electron scattering.

We would like to calculate first the probability $q(x)$, that an electron which is excited at a distance x from the front surface of a photocathode of thickness t , will reach the front surface (at $x = 0$) by electron-phonon scattering only. This may be expressed as a sum

$$q(x) = \sum_{n=0}^{\infty} p_n(x), \quad (A1)$$

in which $p_n(x)$ is the probability that the excited electron will reach the surface by a random walk of n collisions. This probability may be expressed in terms of the probability $p_{n-1}(y)$ (a path of $n-1$ collisions before reaching the surface) by the following recursive integral

$$p_n(x) = \frac{a}{2} \left[\int_0^x p_{n-1}(y) e^{-ay} dy + \int_x^t p_{n-1}(y) e^{-a(t-y)} dy \right], \quad (A2)$$

in which we are able to write explicitly the probability for the excited electron to have its first electron-phonon collision in the differential dy as

$$\frac{1}{2} a e^{-ay} dy \quad \text{for } y < x$$

and

$$\frac{1}{2} a e^{-a(t-y)} dy \quad \text{for } y > x,$$

where c is the total linear cross section for secondary electron scattering, $a + b$.

In these expressions the factor of $\frac{1}{2}$ simply accounts for the likelihood for the excited electron either to be initially heading toward a y position that is less than or greater than x . Thus the first integral in Eq. (A2) is the contribution to $p_n(x)$ of all scatterings for which the first collision is in the volume between x and the front surface, and the second integral is that for which the first collision is in the volume between x and the back surface. Using the definition for $q(x)$ in Eq. (A1) we may now rewrite Eq. (A2) as the following relation:

$$\sum_{n=1}^{\infty} p_n(x) = q(x) - p_0(x) \\ = \frac{a}{2} \left[\int_0^x q(y) e^{-ay} dy + \int_x^t q(y) e^{-a(t-y)} dy \right], \quad (A3)$$

where p_0 is the probability that the electron may reach the front surface without scattering and is given by

$$p_0(x) = \frac{1}{2} e^{-ax}. \quad (A4)$$

By differentiating Eq. (A3) twice with respect to x , we obtain the differential relation

$$q''(x) - a^2 q(x) = 0, \quad (A5)$$

which must have a solution of the form

$$q(x) = A e^{ax} + B e^{-ax}. \quad (A6)$$

Here u is equal to $(c^2 - ac)^{1/2} = (b^2 + ab)^{1/2}$ and A and B are thickness dependent.

We may now obtain A and B by substituting Eq. (A6) into Eq. (A3) (which must yield the same solution for A and B for all values of x between 0 and t). For $x = 0$, we obtain the probability that an electron which is excited at the surface will be heading toward the surface and, if not reflected, will escape, viz.,

$$q(0) = A + B = \frac{a}{2} \left[\int_0^t (Ae^{ux} + Be^{-ux}) e^{-u^2 y} dy \right] + \frac{1}{2}. \quad (\text{A7})$$

And, similarly, for $x = t$, we obtain the probability that an electron which is excited at the opposite surface will reach the surface at $x = 0$ and heading toward this surface, viz.,

$$q(t) = Ae^{ut} + Be^{-ut} = \frac{a}{2} \left[\int_0^t (Ae^{ux} + Be^{-ux}) e^{-u^2 y} dy \right] + \frac{1}{2} e^{-u^2 t}. \quad (\text{A8})$$

Completing the integrals in Eqs. (A7) and (A8), we then use these two equations to solve for A and B , obtaining

$$A = -c\delta / [(u + c)(e^{2ut} - \delta^2)] \quad (\text{A9})$$

and

$$B = ce^{2ut} / [(u + c)(e^{2ut} - \delta^2)]. \quad (\text{A10})$$

where

$$\delta = (c - u)/(c + u).$$

The number of secondaries that are excited at x within a layer dx and per unit area of photocathode surface, can be written as the photon intensity I at x , multiplied by $(E \mu dx / \bar{E})$, according to the simplified model description given above and discussed in more detail in Ref. 10. [$\mu(E)$ is the fraction of the photons that are absorbed per unit volume and $\bar{E}$ is the mean energy of the secondaries.] Therefore, we may write for the x-ray photoemission from the front and back surfaces of a finite photocathode the following quantities to which Y_f and Y_b are proportional, viz., the number of secondaries heading toward and at these surfaces.

$$Y_f \sim E \mu(E) \int_0^t q(x) e^{-u^2 x} dx, \quad (\text{A11})$$

$$Y_b \sim E \mu(E) \int_0^t q(t - x) e^{-u^2 x} dx. \quad (\text{A12})$$

Finally, by substituting into these relations the expressions for A and B given in Eqs. (A9) and (A10) and making the assumption that the x-ray attenuation length $(\mu\rho)^{-1}$ is very large as compared to the escape length u^{-1} , we obtain the x-ray photoemission yields that were quoted in the text's Eqs. (5) and (6), viz.

$$Y_f = K E \mu(E) \frac{c}{u(u + c)} \frac{1 - e^{-u^2 t}}{1 + \delta e^{-u^2 t}} \quad (\text{A13})$$

and

$$Y_b = K E \mu(E) \frac{ce^{-u^2 t}}{u(u + c)} \frac{1 - e^{-u^2 t}}{1 + \delta e^{-u^2 t}}. \quad (\text{A14})$$

The constant K is the fraction of the electrons that are heading toward emission surface and are just inside that surface which do escape. To determine this quantity, appropriate assumptions must be made for the internal secondary electron energy distribution which then allows a determination of the number of electrons with sufficient energy to escape, i.e., of energy greater than a work function or an electron affinity. (The energy distribution is a function of such parameters as the Fermi energy and the band-gap energy.) We may use the one-dimensional analysis described here to define a corresponding isotropic three-dimensional distribution of electron velocities at the surface, conserve the transverse momentum for the escaping electron, and thereby determine the escape cone angle for an electron of a given energy. Integrating this "escape probability" over the allowed angles and energies yields the total escape fraction K . This procedure has been described in Ref. 10.

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1. "Low Energy X-Ray Spectroscopy with Crystals and Multilayers,"
B. L. Henke.
2. "A Sensitometric Calibration of the RAR 2497 Film for the Low
Energy X-Ray Region," E. R. Dietz, T. S. Durland,
B. L. Henke and M. A. Tester.
3. "Low Energy X-Ray Interactions: Photoionization, Scattering,
Specular and Bragg Reflection," B. L. Henke.
4. "Appendix: The Atomic Scattering Factor, $f_1 + if_2$, for 94 Elements
and for the 100 to 2000 eV Photon Energy Region," B. L. Henke,
Ping Lee, T. J. Tanaka, R. L. Shimabukuro and
B. K. Fujikawa.

LOW ENERGY X-RAY PHYSICS PROGRAM

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ABSTRACT

The molecular and sputtered/evaporated multilayers and the acid phthalate crystals can be applied for relatively fast, high efficiency spectral analysis of constant and pulsed low energy x-ray sources in the 100 to 2000 eV region. Limits of resolution are about 1 eV. Reviewed here are the basic methods for the theoretical and the experimental characterization of these analyzers as required for absolute x-ray spectrometry. The design and absolute calibration of spectrographs for pulsed low energy x-ray source diagnostics are described.

1. INTRODUCTION--GRATING VS BRAGG SPECTROMETRY

Generally, the grazing incidence, diffraction grating spectrometry and the large angle Bragg diffraction spectrometry are complementary. Grating spectrographs can yield lower limits of resolution (<0.1 eV) but with relatively small aperture and low dispersion. The crystal/multilayer spectrographs are of higher limits of resolution (>0.5 eV) but with simpler and more flexible large angle geometry and with high dispersion. The crystal/multilayer spectrographs are of large aperture with an overall spectrographic speed that is considerably higher for constant source and somewhat higher for pulsed source spectroscopy. A precise intensity and window profile calibration of the crystal/multilayer instrument is more easily attainable. Having accurately characterized instrument window functions permits an effective resolution enhancement in the crystal/multilayer spectrometry by simple deconvolution procedures. The two spectrographic approaches are clearly complementary, and, ideally, both the grating and the crystal/multilayer spectrographs should be applied for an optimized analysis of many spectroscopic problems. (For a comprehensive review of grating spectrometry, see that by E. Kallne in these Proceedings.)

Even with very intense excitation sources such as some synchrotron/storage ring and high temperature plasma sources, it may be that the crystal/multilayer spectrographs must still be used because the number of photons actually available for proper spectroscopic analysis is limited by other factors. The higher spectrographic speed may be required to achieve satisfactory statistics along with high temporal resolution in time-resolved spectroscopy. Primary monochromators may be required for needed selective excitation of spectroscopic samples which in turn may seriously limit the intensity available for high resolution spectroscopy. Finally, the spectroscopic sample may suffer appreciable radiation damage under the excitation dose that may be required for a given spectrographic measurement. An example of this type of problem is shown in Fig. 1. A low energy x-ray spectral analysis for the molecular orbital configuration of the crystalline solid sample of sodium perchlorate by a relatively fast, flat crystal spectrograph requires approximately three hours for one percent statistics. As shown here, with nine-minute scans through this period, the sample is steadily reduced through successive oxidation states with the last scan revealing the molecular orbital spectrum that is characteristic of NaCl. A successful analysis of this sample was possible [1,2] only by distributing the dosage over eight samples using selective excitation by photons of energy for which the photoionization process that is required has the highest cross section and using time

resolved data collection which permitted an extrapolation to a "zero-dose" spectrum. Resolution enhancement was used to bring the energy resolution of this measurement to about 0.5 eV, using a lead myristate, molecular multilayer analyzer.

CHEMICAL CHANGES

INDUCED BY

 1.75×10^{13} C-K α (277 eV) PHOTONS/SEC-CM 2

Figure 1

For high efficiency, low energy x-ray spectroscopy in the 100-2000 eV region, the sputtered/evaporated multilayers, the molecular multilayers (such as the Langmuir-Blodgett type) and the acid phthalate crystals can be used. The total intensity that may be measured within a diffracted spectral line is proportional to the integrated reflectivity, R , for the given analyzer. In Fig. 2 are plotted the integrated reflectivities for the molecular multilayer, lead myristate, and for the crystal, potassium acid phthalate (KAP), of 2d-values equal to 80 and 26.6 Å, respectively. Suggested here is the fact that this type of molecular multilayer is an excellent analyzer for photon energies below 280 eV (the carbon-K edge) as is the potassium acid phthalate crystal above 530 eV (the oxygen-K edge). For the 300-500 eV region, an appropriately designed sputtered/evaporated multilayer which diffracts this spectral band around 90 degrees from the incident beam direction would be ideal. This requires a 2d-value of about 44 Å for which there are no practical analyzers of the molecular or crystal types at this time.

As discussed elsewhere in these Proceedings by T. Barbee and by E. Spiller, multilayers may be constructed by either sputtering or evaporating in vacuum successive double layers of a variety of low and high atomic number materials. The thickness of the double layer (the d-spacing) may be as small as about 15 Å. It should be feasible to construct spectrographic analyzers of this type that are very effective in the 300-500 eV region.

The molecular multilayers are obtained by successive dipping of a substrate in and out of a trough of water on which is formed an insoluble monomolecular film. [3] Typically, the lead salts of straight-chain fatty acids are used following procedures that were first described by Langmuir and Blodgett. [4,5,6] A schematic which suggests how these layers (Y-type) deposit upon the substrate is presented in Fig. 3. We have made low energy x-ray analyzers of this molecular type from a series of fatty acids that have 2d-values

MOLECULAR MULTILAYER DEPOSITION (Y-TYPE)

Figure 3

Figure 4

INTEGRATED REFLECTIVITY, R LEAD MYRISTATE (200 d-SPACINGS)

THEORETICAL
M-- MOSAIC P-- DARWIN-PRINS

EXPERIMENTAL
• HENKE, et al (1980)

INTEGRATED REFLECTIVITY, R POTASSIUM ACID PHTHALATE (KAP)

THEORETICAL
M-- MOSAIC P-- DARWIN-PRINS

EXPERIMENTAL
— BLAKE, et al (1979)
• HENKE, et al (1980)

Figure 2

LEAD MYRISTATE MOLECULE

Figure 5

in the range of 70 to 160 Å. In Fig. 4 we present the measured 2d-values as a function of the number, n, of CH₂ groups of a lead salt of the straight-chain fatty acids. From this and other crystallographic data, we have constructed a model for the unit cell structure of these systems which is described in Fig. 5 and applied here in a theoretical description of their x-ray reflection characteristics.

The acid phthalate crystals have unit cell structures which have been determined by Okaya [7] and by Smith [8] which we have described and applied in our characterizations of these analyzers as recently reported elsewhere [9]. The practical characteristics of these analyzers are described in detail, experimentally and theoretically, in these Proceedings by R. Blake.

In this review we summarize some of the basic theoretical and experimental methods that may be applied to effectively characterize the crystals and multilayers for well calibrated, low energy x-ray spectrometry. And in the last section we describe spectrographs that have been specially designed for pulsed source diagnostics which utilizes crystal and multilayer analyzers for the low energy x-ray region. Procedures for the application of these spectrographs for absolute, resolution-enhanced spectrometry are outlined.

II. THE THEORETICAL CHARACTERIZATION OF MULTILAYERS AND CRYSTALS FOR THE LOW ENERGY X-RAY REGION

In a companion paper in these Proceedings [10], the author has derived an expression for the analyzer reflectivity for a finite number of diffracting planes using the Darwin-Prins model. The results may be expressed in terms of complex variables in a form that is easily programmed on a small computer for effective crystal/multilayer characterization. We define:

- $I_H(\theta)$: the reflectivity curve (rocking curve)--the ratio of the diffracted intensity to the incident intensity for a plane wave at a grazing angle of incidence and reflection, θ , and for an analyzer of N diffracting layers.
 $I_\infty(\theta)$: the reflectivity curve for an analyzer of an effectively infinite number of diffracting layers (a thick analyzer).
 s : the fractional amplitude, for a plane wave, that is reflected at each diffracting plane.
 σ : the fractional decrease in amplitude of the transmitted beam as it passes through each diffracting plane.
 ξ : a small quantity which measures the phase change of the wave incident at angle θ as it proceeds from one plane to the next ($2nd \sin \theta / \lambda$) through the relation

$$\frac{2nd \sin \theta}{\lambda} = \frac{2nd \sin \theta_0}{\lambda} + \xi = m\pi + \xi, \quad (1)$$

where θ_0 is the angle defined by the Bragg relation, $m\lambda = 2d \sin \theta_0$.

- η : a small quantity that is used to describe the effective attenuation of a wave as it transmits through N layers which dynamically includes all contributions from multiple reflections. The amplitude attenuation factor is x^N , where $x = (-1)^{m_0} \eta$ and

$$\eta = \pm \sqrt{s^2 - (\xi + \sigma)^2} \quad (2)$$

with + or - sign chosen so that the real part of η is greater than zero.

We may then write [9]

$$I_H = I_\infty |1 - e^{-2N\eta}|^2, \quad (3)$$

where

$$I_\infty = \left| \frac{-s}{(\xi + \sigma) \mp \sqrt{(\xi + \sigma)^2 - s^2}} \right|^2, \quad (4)$$

where the + or - sign is chosen so that $I_\infty < 1$.

As described in the companion paper, σ and s can be calculated in terms of the average atomic scattering factor per unit volume, $\bar{n}$, and the structure factor per unit volume, ϕF , through the relations

$$\sigma = -r_0 \lambda d \frac{\bar{n} F}{\sin \theta} \quad (5)$$

and

$$s = -r_0 \lambda d \frac{\phi F}{\sin \theta} P(2\theta) \quad (6)$$

where r_0 is the classical electron radius and for the low energy x-ray region, $\bar{n} F$ and ϕF can be readily calculated given the structure of the multilayer or crystal system and using the tabulated atomic scattering factors as presented in the Appendix of these Proceedings. In the companion paper [10], $\bar{n} F$ is given by Eq. (5) and (6), and ϕF is given by Eqs. (32) and (33) for crystals and molecular multilayers and by Eqs. (34) and (35) for the sputtered/evaporated multilayers.

It should be noted that the diffraction order number, m , and the polarization factor $P(2\theta)$ are introduced through the reflection parameters, F and s . For an incident wave of electric vector in the plane of diffraction, $P(2\theta)$ is equal to $\cos 2\theta$ and for the electric vector perpendicular to the plane of diffraction, $P(2\theta)$ is equal to unity. For incident, unpolarized light, therefore, the corresponding unpolarized components, I_σ and I_π , are combined as

$$I_H(\theta) = \frac{1}{2}(I_\pi(\theta) + I_\sigma(\theta)).$$

It may be shown that the dynamical model relation for $I_H(\theta)$ given here in Eqs. (3) and (4) will reduce to the usual kinematical approximation for the analyzer of such low scattering and absorption within the layers that the incident intensity may be assumed to be the same at each plane for the given number of planes, N. Thus by assuming σ and s to be very small, $I_H(\theta)$ becomes

$$I_H = \left| \frac{s(1 - e^{-2N\xi})}{2\xi} \right|^2.$$

Multiplying by the complex conjugate to obtain this modulus squared, and letting ξ be replaced by $\sin \xi$ in the denominator since ξ is necessarily a small quantity for θ near the diffraction peak, we obtain for unpolarized incident radiation

$$I_H = (r_0^2 \lambda^2 d^2) \frac{(\phi F_\pi)^2 + (\phi F_\sigma)^2}{\sin^2 \theta_0} (1 + \cos^2 2\theta) \frac{\sin^2 N\xi}{\sin^2 \xi}. \quad (7)$$

Because this diffraction peak will be relatively sharp, the parameter, ξ , may be written from Eq. (1) as

$$\xi = \frac{2\pi d}{\lambda} (\sin(\theta_0 + \Delta\theta) - \sin \theta_0) = \frac{2\pi d}{\lambda} \cos \theta_0 \Delta\theta \quad (8)$$

and this kinematical description will assume the familiar form [12]

$$I_H(\Delta\theta) \sim \frac{\sin^2 \left(\frac{2\pi Nd}{\lambda} \cos \theta_0 \Delta\theta \right)}{\sin^2 \left(\frac{2\pi d}{\lambda} \cos \theta_0 \Delta\theta \right)}. \quad (9)$$

Applying the Rayleigh criterion, we define a limit of angular resolution as that $\Delta\theta_1$ which corresponds to the first minimum of this diffraction pattern. Therefore

$$\frac{2\pi Nd}{\lambda} \cos \theta_0 \Delta\theta_1 = \pi \text{ and } \Delta\theta_1 = \frac{\lambda}{2Nd \cos \theta_0}.$$

Using the Bragg relation $m\lambda = 2d \sin \theta_0$ and its derivative, we may then find the corresponding wavelength resolution as

$$\Delta\lambda = \lambda/mN \quad (10)$$

and finally, by definition, the resolving power of this analyzer of low attenuation becomes

$$\frac{\lambda}{\Delta\lambda} = mN = \frac{E}{\Delta E} \quad (11)$$

This resolving power is then an upper limit that may be expected of a multilayer of a relatively small number of layers, N , and at diffraction order, m .

For some analyzers, particularly for very low energy x-rays and with sputtered/evaporated multilayers, the effective number of diffracting planes may be limited by absorption within the multilayer and the dependence upon N drops out for N sufficiently large but finite. If then we consider the absorptive parameter, α , to be large as compared with the reflective parameter, s , the reflectivity curve, $I_H(\theta)$, from Eq. (3), becomes the Lorentzian function

$$I(\theta) = \frac{\left(\frac{\omega}{2\pi}\right)P_m}{\left(\Delta\theta - \frac{\delta}{\sin\theta_0 \cos\theta_0}\right)^2 + \left(\frac{\omega}{2}\right)^2} = \frac{\left(\frac{\omega}{2\pi}\right)P_m}{\epsilon^2 + \left(\frac{\omega}{2}\right)^2} \quad (12)$$

This function will have its peak value displaced from the Bragg angle, θ_0 , by an amount equal to $\delta/\sin\theta_0 \cos\theta_0$, which is a refraction shift of the diffraction pattern that may also be predicted by combining the Bragg relation with Snell's law [11,12]. It is interesting to note that this result follows here for the case of relatively high absorption within the analyzer. For this Lorentzian rocking curve approximation, its parameters may be written as follows:

The angle, ϵ , as measured from the diffraction peak

$$\epsilon = \Delta\theta - \delta/\sin\theta_0 \cos\theta_0 \quad (13)$$

The full-width-at-half-maximum (FWHM)

$$\omega = 2\delta/\sin\theta_0 \cos\theta_0 \quad (14)$$

The corresponding integrated reflectivity (area under the Lorentzian) for unpolarized incident radiation

$$R_m = \frac{r_0^2 \lambda^4}{16\pi\beta} [(\phi F_1)^2 + (\phi F_2)^2] \frac{1 + \cos^2 2\theta}{\sin 2\theta} \quad (15)$$

Here the optical constants, δ and β , are as have been defined in Ref. 10 of these Proceedings to be given by

$$\delta = \frac{r_0 \lambda^2}{2\pi} n\bar{F}_1 \quad (16)$$

$$\beta = \frac{r_0 \lambda^2}{2\pi} n\bar{F}_2$$

The integrated reflectivity, R_m , that results from this Lorentzian, absorption-limited approximation, is identical to that which may be obtained from the mosaic crystal model [11,12] and as given in Ref. 10.

According to the mosaic crystal model, we may include the effect of a finite crystal thickness by multiplying the expression for R_m in Eq. (15) by the factor

$$(1 - \exp(-2\mu t/\sin\theta_0))$$

In which μ is the mass photoionization cross section for the crystal material, ρ is the average mass density and t is the crystal thickness which is approximately equal to $1/d$. If the crystal or multilayer has a significant mosaic quality, the FWHM of its rocking curve will be greater than that expected from the perfect crystal model and will normally be determined by measurement. As is illustrated in Fig. 2, this integrated reflectivity, R_m , generally tends to be higher than R_p , that as derived by numerically integrating for the area under $I_H(\theta)$ from Eq. (3). Well defined crystals such

as the acid phthalates, for example, will typically have experimentally measured values for the integrated reflectivity that fall between these values for the mosaic and the perfect crystal models.

As has been discussed in the companion paper of these Proceedings [10], this relatively simple Darwin-Prins model approach for the characterization of low energy x-ray analyzers is generally in good agreement with the rigorous E & M boundary values approach (the characteristic matrix approach) for the perfect multilayer systems. [13,14] Generally, the approximations that are inherent in the Darwin-Prins approach for the finite crystal/multilayer system as has been described here are appropiate inasmuch as the typical real crystal/multilayer system cannot be defined any more precisely than is this approximate model. In the design of low energy x-ray analyzers, particularly of the sputtered/evaporated type, this simple theoretical model can provide helpful, immediate insights as to the interplay of the electron scattering contrast yielded by the structure factors and the multilayer absorption, and their effect upon the analyzer performance. In Fig. 6 the integrated reflectivity, R_m , from the thick mosaic model, has been plotted for photon energies above the C-K edge and for a variety of practical sputtered/evaporated, equal-thickness double layers of d equal to 30 Å. For these calculations, structure factors were used as for sharply defined interfaces between the 15 Å layers. As has been discussed in the companion paper [10], the integrated reflectivities would be significantly reduced if a graded-density or rough interface were to be involved.

INTEGRATED REFLECTIVITY, R ,

FOR
SPUTTERED OR EVAPORATED MULTILAYERS
WITH
15 Å EQUAL THICKNESS LAYERS -- $2d = 60$ Å

- (A) TUNGSTEN/BORON
- (B) TUNGSTEN/CARBON
- (C) MOLYBDENUM/CARBON
- (D) MOLYBDENUM/TITANIUM
- (E) TITANIUM/CARBON

Figure 6

In Fig. 7 we compare the diffraction peak profiles for the lead myristate molecular multilayer and the tungsten-carbon sputtered/evaporated multilayer with the same $2d$ -value of 80 Å. Here the fractional thickness of the d -spacing for the heavy layer (tungsten), defined as Γ , is varied. Again a sharply defined interface was assumed for the W/C multilayer which yields appreciably higher predicted peak intensities than are observed relative to those for the lead myristate. The measured angular widths of the rocking curves are in good agreement with these as predicted, however.

III. THE EXPERIMENTAL CHARACTERIZATION OF MULTILAYERS AND CRYSTALS FOR THE LOW ENERGY X-RAY REGION

The optimized low energy x-ray analyzer will have the maximum, effective number of layers as determined essentially by the crystal/multilayer attenuation. (N for the multilayers chosen sufficiently large.) For such analyzers the perfect crystal model relation, $I_{\omega}(0)$, presented here in Eq. (4), predicts a diffraction curve with Lorentzian wings. That is, for angles not close to the peak, ξ becomes relatively large as compared with σ and s and the intensity distribution falls off as $(\Delta\theta)^{-2}$ as for a Lorentzian. As already noted above, for many practical crystals and multilayers applied in the high attenuation, low energy x-ray region, the total profile tends to become Lorentzian.

In Ref. 9 we have calculated in detail the reflectivity characteristics vs photon energy for five acid phthalate analyzers and five each of 100-layer molecular and sputtered/evaporated (tungsten-carbon) multilayers. For such characterizations, we define the integrated reflectivity as the area under the reflectivity curve within the limits of plus/minus 5ω , (at which limits $I_H(\theta) \approx .01$). We have compared the integrated reflectivity as obtained by precise numerical integration under the theoretical reflectivity curve to that for a Lorentzian curve having the same FWHM, ω , and the same peak height as that given by $I_H(0)$. The two integrated reflectivities generally agree within ten percent. Finally, our measured molecular and sputtered/evaporated multilayer rocking curves, after correcting for instrumental broadening, are well described by Lorentzian fits. Similarly it has been found that the reflectivity curves for the acid phthalate crystals may be described as Lorentzian. [15]

In our experimental characterization of low energy x-ray analyzers, therefore, we assume that the reflectivity curve is essentially Lorentzian which may be then described by the relation

$$I(\epsilon) = \frac{(\omega/2\pi)R}{\epsilon^2 + (\omega/2)^2} \quad (17)$$

A. THE MEASUREMENT OF THE FWHM- ω

Our measurements of ω for a given analyzer are of a series of monochromatic line sources which are Lorentzian in their wavelength and photon energy distribution and produce an equivalent angular broadening of the spectral line equal to ϵ_0 . A conventional, flat crystal spectrograph is used with soller slit collimation that presents a further angular broadening of a Gaussian shape and of FWHM equal to g . Pulse height discrimination is utilized with a flow proportional counter to minimize background under the isolated spectral line.

The convolution of Lorentzians yields another Lorentzian with the widths adding linearly. The convolution of Gaussians yields another Gaussian, but with the widths adding quadratically. Because in many spectroscopic measurements the collimation is Gaussian, the measured spectral line is the result of a convolution of a Gaussian collimation function with a Lorentzian analyzer plus emission line profile. The Gaussian-Lorentzian convolution yields a Voigt curve for which there is no exact analytical function

COMPARISON OF MOLECULAR AND SPUTTERED/EVAPORATED MULTILAYERS AT Mo-M α_1 (64.4 Å/192.3 eV)

Figure 7

description.

We have shown [1] that within a sufficiently good approximation, the Voigt function can be described simply as a linear mixing of the two basic broadening functions, the Gaussian, $G(x)$, and the Lorentzian, $L(x)$ through the relation

$$V(x) = \delta G(x) + (1 - \delta)L(x). \quad (18)$$

If we define the FWHM widths for the Gaussian, the Lorentzian and their fold, the Voigt function by g , l and v , respectively, and the variable x by ϵ/v (ϵ is the angle from the peak), we may then write

$$G(x) = e^{-(\pi/2)x^2} \text{ and } L(x) = \frac{1}{1+x^2} \quad (19)$$

and the mixing parameter, δ , becomes

$$\delta = 1 - l/v = (g/v)^2. \quad (20)$$

In our crystal characterizations, l represents the sum of the Lorentzian crystal multilayer and emission line widths, $\omega + \epsilon_0$, and we may write for the analyzer width, ω , from Eq. (20)

$$\omega = v(1 - (g/v)^2) - \epsilon_0. \quad (21)$$

These numerically derived relationships have been tested on a series of low energy x-ray emission lines for which the natural widths have been precisely measured using photoelectron spectroscopy. [1] We illustrate in Fig. 8 how the Mo-M α_1 (64.4 Å/192.3 eV) line is used to determine the lead myristate molecular analyzer diffraction width, ω , to be 0.33° and, equivalently, in energy width, 0.82 eV. These values may be compared with those as determined from the theoretical reflectivity curve, $I_H(0)$, given in Eq. (3) to be 0.36° and 0.89 eV, respectively.

B. THE MEASUREMENT OF THE INTEGRATED REFLECTIVITY, R

Practical flat crystal calibration for the integrated reflectivity, R , usually involves incident beams which are neither precisely monochromatic nor parallel. Let the incident beam be of cross section that is smaller than the window area of the detector and be of total direct beam intensity P_0 counts per second. Consider the beam to be made up of a collection of rays with a narrow distribution of angular divergence about a central ray and each with intensity, ΔP_n . The intensity that is reflected for the n th ray near a θ incidence angle is ΔP_n . Then if $I_H(0)$ is the reflectivity, we may write

MOLYBDENUM-M_α (54.54/192.3 eV)
AS MEASURED BY A
LEAD MYRISTATE ANALYZER (2d=79.9 Å)

Figure 3

$$\Delta P_n = \Delta P_{on} I_n(\theta) .$$

Let the crystal be rotated through a range in θ that completely embraces a diffraction peak for all incident rays and at an angular rate of ω_c . If dE_n is the total counts measured by the detector for the n th ray during interval dt , we may write

$$dE_n = \Delta P_{on} I_n(\theta) dt = \Delta F_{on} I_n(\theta) (d\theta/\omega_c)$$

and

$$\Delta E_n = (\Delta P_{on}/\omega_c) \int I_n(\theta) d\theta = (\Delta P_{on}/\omega_c) R .$$

Now summing over all n rays in the divergent incident beam, we obtain the total counts collected, E , as a diffraction peak is scanned as

$$E = \sum_n \Delta E_n = \frac{1}{\omega_c} R \sum \Delta P_{on} = \frac{P_0 R}{\omega_c} .$$

And thus R may be expressed in terms of measurable quantities as

$$R = \frac{E \omega_c}{P_0} . \quad (22)$$

If the incident beam is not precisely monochromatic, but consists of a narrow band of wavelengths about a mean value, a similar argument as presented above may be applied to yield the same result as Eq. (22), where R would then represent an integrated reflectivity characteristic of an average wavelength. This follows from the fact that the intensity distribution for a variable wavelength component is simply shifted a small amount in angle according to the Bragg relation--but still embraced in the complete scan taken over the diffraction peak. The value of R thus determined is independent of a small departure from monochromaticity of the beam--providing that the reflectivity is slowly varying over the spread in wavelengths involved.

In Figs. 9 and 10 we have applied this flat crystal calibration procedure in order to compare the performance of a molecular and a sputtered multilayer in the 500-1000 eV photon energy region. The sputtered multilayer, constructed by T. Barbee, has a 2d-value of 44.2 Å, $N = 62$, and $\Gamma = 0.3$. The molecular multilayer is lead myristate of 2d equal to 80 Å and $N = 200$. These comparative spectral scans of characteristic line radiations were taken with soller slit collimation of Gaussian, FWHM value, g , equal to 0.34 in θ -coordinates. The multilayer angular width, FWHM- ω , was determined using Eq. (21), its integrated reflectivity determined by Eq. (22) and the percent peak reflectivity, P , assuming a Lorentzian reflectivity curve as in Eq. (17), and equal to $[2R/\pi\omega] \times 100$.

With calibrated crystal/multilayer analyzers, and instrument collimation window functions, and with the measured spectral line widths, Eq. (21) may then be used to determine the emission line width with enhanced resolution. We have developed a simple method for treating overlapping spectral lines [1] by fitting a sum of Voigt functions as given in Eq. (18) by a Simplex method which fitting determines the angular position, weight and width of each component lines in the overlapping spectrum. Eq. (21) is then used to determine the individual emission line widths. Again, enhanced resolution is obtained.

Often, rather than flat crystal optics with essentially parallel incident radiation, divergent beam optics (as with Johann circle geometry) or with non-focussing optics for an instantaneous presentation of an emitted spectrum (for pulsed source spectroscopy) may be used. For spectrographs using these divergent beam geometries, the measured intensity profiles for a monochromatic source may usually be predicted in terms of the flat-crystal reflectivity characteristic parameters and appropriate geometric factors. This is illustrated in the next section for the pulsed source spectrographs which utilize the cylindrical-convex crystal/multilayer and the elliptical crystal/multilayer.

IV. PULSED SOURCE SPECTROSCOPY

A. THE CONVEX CYLINDRICAL CRYSTAL ANALYZER

The convex cylindrical crystal [3,16-20] presents to an x-ray source a continuum of reflecting regions with Bragg angles beginning from zero value. For a particular wavelength, the effective aperture is proportional to $\sin\theta$ and hence to λR for the usual application geometry in which the cylinder radius, r , is small as compared with the distance to the source, s . We have constructed cylindrical analyzers of good quality by bending .005" cleaved sections of KAP to radii as small as one inch, and by dipping polished cylinder substrates of radii as small as a few millimeters to generate the Langmuir-Blodgett type of molecular multilayers. The

CHARACTERIZATION OF BRAGG ANALYZERS

Figure 9

COMPARISON OF MULTILAYER ANALYZERS--500-1000 eV REGION

TUNGSTEN-CARBON--62 11-PLUS-11 d-SPACINGS--2d=44.2 Å

LEAD MYRISTATE--200 d-SPACINGS--2d=80 Å

ROCKING CURVE FWHM-- ω (°) AND W(eV)

REFLECTIVITY--INTEGRATED, R(mv) PEAK, P(%)

COLLIMATION FWHM (GAUSSIAN)--0.77° (2θ)

Figure 10

sputtered/evaporated multilayers may be deposited upon a flat, flexible substrate which may then be bent to a desired radius.

Some useful geometrical relations which characterize this analyzer are as follows (see Fig. 11):

$$\cos \theta = \cos \chi - (1/\delta) \sin \chi \quad (23)$$

and

$$(dx/d\theta) = \delta \sin \theta / (\delta \sin \chi + \cos \chi) \quad (24)$$

in which $\delta = r/s$. Now for $\delta \ll 1$, it follows that

$$\cos \theta = 1 - \chi/\delta \quad (25)$$

and

$$(dx/d\theta) = \delta \sin \theta \quad (26)$$

To relate the reflecting region position, α , with the corresponding Bragg angle, θ

$$\alpha = \theta - \chi = \theta - \delta(1 - \cos \theta). \quad (27)$$

And to relate the position of the detector, β , to the corresponding Bragg angle, θ --for $r \ll R$ (crystal-detector distance)

$$\beta = 2\theta - \chi = 2\theta - \delta(1 - \cos \theta). \quad (28)$$

And, finally, for instruments with $\delta \ll 1$, a relation between the divergent beam diffraction line profile, $dN/d\theta$, defined as $P(\theta)$, produced by the cylindrical crystal and the parallel beam, flat crystal reflectivity ratio, $I_N(\theta)$, can be obtained as

$$\frac{dN}{d\theta} = P(\theta) = I(\theta) \{i_0 a \psi\} (dx/d\theta) = \delta i_0 a \psi \sin \theta \quad (29)$$

where i_0 is the number of photons per sec-unit source area-stereadian, a is the source slit area, and ψ is the angle at the source slit as subtended by the crystal width, and assuming the slit thickness to be negligible.

The total number of photons, N , within the diffraction line profile is proportional to the crystal's integrated reflectivity, R , and given by

$$N = \int P(\theta) d\theta = \delta i_0 a \psi \sin \theta / I(\theta) d\theta = \delta (i_0 a \psi \sin \theta) R. \quad (30)$$

Finally, to determine the effect of slit or line source width upon the profile, we integrate the differential intensity from a section of the slit of width, b , and differential thickness, $sd\phi$, (as reflected into the diffraction line profile) within the limits $-\phi_0$ to $+\phi_0$, where $2\phi_0$ is the angular thickness of the slit as measured at the crystal. We obtain, assuming $I_N(\theta)$ to be Lorentzian, as given in Eq. (17):

$$P'(\theta) = \{ \delta i_0 b s \sin \theta \} \left(\frac{\omega}{2\pi} R \right) \int_{-\phi_0}^{\phi_0} \frac{d\phi}{(\epsilon - \phi)^2 + (\omega/2)^2}.$$

CYLINDRICAL CRYSTAL GEOMETRY

Figure 11

Thus

$$P'(\theta) = \{i_0 b s \sin \theta\} \left\{ \frac{R}{\pi} \right\} \left(\tan^{-1} \frac{E + \phi_0}{\omega/2} - \tan^{-1} \frac{E - \phi_0}{\omega/2} \right) \quad (31)$$

$P'(\theta)$ has been plotted for several relative values of ϕ_0/ω in Fig. 12. If the source brightness, i_0 , is not uniform but rather is a function of ϕ , then $i_0(\theta)$ must be folded within the integral.

B. THE ELLIPTICAL CRYSTAL/MULTILAYER SPECTROGRAPH

Shown in Fig. 13 are the basic features of the proposed spectrograph for the spectral analysis of a pulsed low energy x-ray source. An elliptically curved crystal or multilayer analyzer is utilized with an effective point or line source at or through one of the foci and a small exit aperture (scatter aperture) at the second focal point. The elliptical analyzer curvature may be a cylindrical section, or it may be of double curvature and as a surface of revolution about the major arcs (an ellipsoidal section).

Considerable importance in the design of this spectrograph [21] has been placed upon achieving a minimum of background radiation and presenting a spectrum that can be simply and accurately interpreted to yield the source spectral characteristics in the low energy x-ray region. The small scatter aperture into the detector module effectively eliminates the stray radiation that may diffusely scatter or fluoresce from the analyzer. An optically flat or cylindrically curved total-reflection mirror with an adjustable entrance slit along with an appropriate filter is used for an effective attenuation of high-order diffracted and the lower-energy radiation background. If the slit at the mirror is adjusted for a sufficiently small entrance aperture, a one-dimensional spatial distribution of the source intensity for the particular wavelength can be presented along the length of a corresponding spectral line for an extended source (spatial resolution in the tenth milliradian range). The spectrum is formed by a relatively small analyzer dimension normal to this drawing section so that the analyzers can thus be "stacked" for multiple band spectral coverage. This is described in Fig. 14.

The elliptically curved crystal/multilayer substrates have been made by computer controlled milling and by computer controlled diamond turning of aluminum blanks. [22] The acid phthalate cleaved sections of about .005" thickness and coverslip glass of about .010" thickness are epoxied to the curved surfaces under

light pressure. The molecular multilayers are deposited directly upon the coverslip glass curved surfaces. The coverslip glass pieces are preformed in an oven to fit a graphite substrate of identical shape as the aluminum substrates.

The diffraction geometry is shown in Fig. 15. In order to establish a focal point for radiation from a small source and thereby an effective scatter aperture, the analyzer curvature is that for the ellipse

$$\rho = \frac{h}{1 - e \cos \beta} \quad (32)$$

where e is its eccentricity and h is the characteristic radial distance, ρ , from the exit focal point for $\beta = \pm 90^\circ$.

An important design feature is that the measured radiation can be normal to a circular arc detection surface (a film surface for photographic detection, a CCD array for electronic detection and for time-resolved spectroscopy, and for a proportional counter goniometer circle in a calibration chamber.) The angular position on this detection circle, θ , is related to the Bragg reflection angle off the analyzer, θ , by the equation

$$\theta = \tan^{-1} \left(\frac{1 - e \cos \beta}{e \sin \beta} \right) \quad (33)$$

which reduces to simply

$$\theta = \beta/2 \quad (34)$$

for applications with a large source distance (i.e., with an eccentricity, e , equal to unity for an approximately parabolic analyzer.

EFFECT OF SOURCE SIZE ON CYLINDRICAL CRYSTAL LINE PROFILE

Figure 12

PULSED X-RAY SOURCE SPECTROSCOPY

ELLIPTICALLY CURVED ANALYZING CRYSTAL

Figure 13

In Fig. 15 we define the angular position of a ray from the source, x , which is related to θ and β by

$$x = 2\theta - \beta \quad (35)$$

and thus differentially

$$\frac{dx}{d\theta} = 2 - \frac{d\beta}{d\theta} \quad (36)$$

And from Eq. (33) we may obtain $d\beta/d\theta$ as

$$\frac{d\beta}{d\theta} = \frac{e^2 + 1 - 2e \cos \theta}{e(1 - \cos \theta)} \quad (37)$$

We would like next to write an expression for the spectral line profile as diffracted by the elliptically curved analyzer of cylindrical section in terms of the flat crystal characteristic parameters, R and ω . As we have described above for the convex, cylindrical analyzer, we shall define by dN the number of photons per sec diffracted by the elliptical analyzer within a differential angular region, $d\theta$, about a Bragg angle, θ , and equal to $P(\theta)d\theta$. Thus the divergent beam angular distribution of intensity as diffracted by the elliptically curved analyzer becomes

$$\frac{dN}{d\theta} = P(\theta) = i_0 a \psi \frac{dx}{d\theta} I_N(\theta) \quad (38)$$

where a is the projected source area; ψ is the angular width of the beam that is accepted by the analyzer and measured in the plane normal to the Bragg reflection plane; and $I_N(\theta)$ is the flat-crystal rocking curve, the fraction of the intensity for a parallel incident beam that is reflected at an angle, θ . Integrating Eq. (38) through the reflecting region in θ for a given wavelength, we obtain the total number of photons per second within the diffracted line as

$$N = i_0 a \psi \left(\frac{dx}{d\theta} \right) \int I_N(\theta) d\theta = i_0 a \psi \left(\frac{dx}{d\theta} \right) R \quad (39)$$

Finally, if we assume that the flat crystal, parallel beam rocking curve, $I_N(\theta)$, to be Lorentzian as in Eq. (17), we may write for $P(\theta)$

$$P(\theta) = i_0 a \psi \left(\frac{dx}{d\theta} \right) \frac{(\omega/2\pi)R}{\epsilon^2 + (\omega/2)^2} \quad (40)$$

where ϵ is measured from the position of the diffracted peak in θ -coordinates. Eq. (40) may be expressed in β -coordinates, as measured along the detection circle, by multiplying the numerator and denominator of the Lorentzian by $(d\epsilon/d\beta)^2$. Here, $d\beta/d\theta$ and $dx/d\theta$ may be

THREE-BAND SPECTROGRAPH USING "STACKED" ANALYZERS

MIRROR*	FILTER	ANALYZER
SiO ₂	CARBON	LEAD BEHENATE 2d-120 Å
SiO ₂	Al ₂ O ₃	LEAD LAURATE 2d-70 Å
SiO ₂	ALUMINUM	KAP 2d-26.6 Å

*FUSED QUARTZ OR PYREX

Figure 14

expressed in variable β through Eqs. (36) and (37). We have defined by $d\beta$ the angular position as measured from the peak position along the detection circle for the Lorentzian defined as follows:

$$d\beta = \left(\frac{d\beta}{d\theta} \right) \epsilon \quad (41)$$

and its measured FWHM, ϕ ,

$$\phi = \left(\frac{d\beta}{d\theta} \right) \omega \quad (42)$$

The β -position for a peak of wavelength λ is obtained by inverting Eq. (33) for the refraction-shifted peak position in θ -coordinates, viz., (from Eq. (12))

$$\theta_0 + \frac{\delta}{\sin \theta_0 \cos \theta_0}$$

In Figs. 16, 17 and 18 are presented plots of our calculated reflectivity characteristics [9] for the three analyzers, lead behenate, lead laurate and potassium acid phthalate of $2d$ -values of 120, 70 and 26.6 Å, respectively. We have proposed these analyzers for a three-band spectrograph for the 100-1000 eV region which has been described in Fig. 13.

In order to verify the response functions for the elliptical spectrograph as predicted here and to account for possible individual differences between the curved crystal/multilayer and the corresponding flat analyzers (on which the flat crystal characteristics have been directly measured), we measured the elliptical

ELLIPTICAL ANALYZER GEOMETRY

Figure 15

LEAD BEHENATE

Figure 16

LEAD LAURATE

Figure 17

analyzer response function directly at a few standard wavelengths by introducing a calibrated low proportional counter, with a precision goniometer, on the detection circle. In this way the diffraction peak is measured in β -coordinates and compared with the directly measured i_0 for a characteristic line source that is filtered and isolated with pulse-height discrimination. Such a spectrum including several orders of the Cu-L α (13.3 A/930 eV) is illustrated in Fig. 19.

To complete an absolute calibration of this spectrograph, it is necessary to include the response of the detector that is utilized. For many applications, an appropriate photographic film is used to time integrate the pulsed spectrum. We calibrate the film material by taking a series of known exposures with the film along the detection circle under the identical conditions with which a corresponding calibrated proportional counter scan has been made (as shown in Fig. 19). The exposed films are microdensitometered with a slit width that is comparable to that on the proportional counter and small as compared to that of the width of the diffraction lines. The measured densities are correlated with the measured photons/microns² exposures for the precisely known wavelength for the spectral line. The calibration of the RAR 2497 film by this procedure is described elsewhere in these Proceedings.

For many pulsed x-ray sources there may be high energy components that diffract effectively in the higher orders and make more difficult a quantitative spectral analysis. In the design of the elliptical analyzer spectrograph as described here, we have used total reflection mirror monochromators to effect the needed high-energy cut-off. We present here in Figs. 20-24 the reflectivity curves for five practical x-ray mirror monochromators which we have calculated using the methods that have been presented in the companion paper.[10] The data presented here, along with some examples of corresponding experimental data, are for mirror surfaces of beryllium, carbon, fused quartz, nickel and gold.

In the low energy diagnostics of essentially point sources (as laser-produced from microballoon sources), it is suggested here that each wavelength component will be presented in either θ or β coordinates as essentially a Lorentzian spectral component of FWHM equal to ω or ϕ , respectively. If the emission line has a distribution of wavelengths because of Doppler and/or Stark broadening, the measured spectral line profile is then a convolution of these and the analyzer broadening functions. Because Doppler broadening is essentially Gaussian and Stark broadening is essentially Lorentzian, a simple resolution enhancement procedure may be possible using that described above and in Ref. 1. The Voigt function fitting may need to be limited to the wings of the spectral lines if, for example, self-absorption effects have reduced the central part of the

POTASSIUM ACID PHTHALATE

Figure 18

Q-L SERIES SPECTRA ($L_{\alpha 2} = 13.336 \text{ \AA}$ $L_{\alpha 1} = 13.053 \text{ \AA}$ $L_{\beta 1} = 15.286 \text{ \AA}$)

Figure 19

REFLECTIVITY OF BERYLLIUM MIRROR ($\rho = 1.85 \text{ gm/cm}^3$)

Figure 20

REFLECTIVITY OF NICKEL MIRROR ($\rho = 8.90 \text{ gm/cm}^3$)

Figure 23

REFLECTIVITY OF CARBON MIRROR ($\rho = 1.54 \text{ gm/cm}^3$)

Figure 21

REFLECTIVITY OF GOLD MIRROR ($\rho = 19.32 \text{ gm/cm}^3$)

Figure 24

REFLECTIVITY OF FUSED QUARTZ MIRROR ($\rho = 2.20 \text{ gm/cm}^3$)

Figure 22

ONE-DIMENSIONAL IMAGING

Figure 25

spectral line.

This elliptical analyzer spectrograph may be effectively applied to extended sources in order to obtain spatially resolved spectral information. In this application, the exit slit of the spectrograph becomes a limiting aperture which accepts radiation only from a linear region of the source perpendicular to the Bragg reflection plane and through the source focal point. If a vertical slit of sufficiently small width is positioned between the source focal point and the analyzer (for example at the total reflection monochromator) imaging along this linear source region occurs at nearly constant magnification along the length of the spectral line (see Fig. 25). Alternatively, this one-dimensional imaging can be obtained with larger instrument aperture by replacing the flat monochromator mirror and limiting slit by a cylindrical mirror of such curvature as to focus the radiation from a point along the accepted line source region to a corresponding point along the spectral line.

In summary, the elliptical spectrograph has three distinct advantages over the convex or flat crystal instruments for presenting an instantaneous spectrum of pulsed x-ray source. These result from the collecting and focussing into a line image within an exit aperture of radiation from a point or line source, and are:

(1) the effective aperture for a given wavelength can be appreciably larger; (2) the detector circle is shielded from the total analyzer area by the exit slit acting as a scatter aperture, thus allowing a considerable reduction in background resulting from diffuse and fluorescent scatter; and (3) the sharp line image within the exit aperture allows a precise definition of the detection geometry (for example, for a film circle for a slit window of a streak camera), making possible a straightforward and accurate absolute calibration.

Finally, it should be emphasized here that for optimized low energy x-ray spectroscopy it is important to choose the 2 θ -values of the analyzers that are comparable to the wavelengths to be measured in order to place the desired spectral bands at the largest possible Bragg angles. At these large angles, the relative effects upon spectral resolution resulting from crystal and source size broadening are minimized because of the higher dispersion. Equally important for the low energy spectroscopy is that only at the larger angles will the Bragg reflection reflectivity of the analyzer be large as compared to its specular reflectivity. At the smaller angles, below about 20° in Bragg angle, the specular reflection tail for the longer wavelengths can represent an appreciable background at the diffraction line. It is for this reason that in the elliptical spectrograph design described here, the spectral bands to be measured are placed at θ -angles from 45° to 135°.

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ABSTRACT

For the low energy x-ray region of 100-2000 eV, the complete atomic interaction, coherent scattering and photoelectric absorption can be described by a complex scattering amplitude which may be given through the atomic scattering factor, $f_1 + if_2$. For this low photon energy region, it is shown by the relativistic quantum dispersion theory that the atomic scattering factors can be uniquely determined from simple relations involving only the atomic photoionization cross section dependence upon photon energy. We have compiled "state of the art" tables for the photoionization cross sections for 94 elements and for the photon energy region of 30-100,000 eV. With this compilation, we have established atomic scattering factor tables for the 100-2000 eV region. By a summing of the complex, atomic scattering amplitudes, a low energy x-ray interaction can be determined. Even for atoms in the molecular or solid state the scattering cross sections remain atomic-like except for photon energies very near the threshold. Using practical examples, the methods of calculation, with the atomic scattering factors, are reviewed here for the following: 1) x-ray energy deposition within materials (energy response of x-ray photocathodes); 2) transmission through a homogeneous medium: refraction; 3) transmission through a random collection of uniform spheres: low angle scattering in an inhomogeneous medium; 4) specular, Fresnel reflection (total and large angle reflection) at smooth boundary; and 5) Bragg reflection from a periodic, layered system--(reflection by crystals and multilayers).

1. INTRODUCTION--THE ATOMIC SCATTERING FACTORS

In this review, we would like to discuss, for the low energy x-ray region (100-2000 eV region), how the interactions of absorption, scattering and reflection can be well described by using the atomic scattering factors as the primary parameters for the material system. In the Appendix of these proceedings we present tables for the atomic scattering factors as directly derived from a recent work [1] on a "state of the art" compilation of the photoionization cross sections for 94 elements for the 30-100,000 eV region, along with the calculated atomic scattering factors for the 100-2000 eV photon energy region. We present here, as applied to selected examples of relevance in low energy x-ray diagnostics, some basic procedures for predicting low energy x-ray interactions.

The interaction physics for the conventional x-ray region (for photon energies above 1000 eV) has been presented by many excellent texts including that of Compton and Allison [2] and R. W. James [3]. What is summarized here is an extension and specialization of this physics that is useful for the long wavelength x-ray region of 10-100 Å.

For the low energy x-rays, the interaction can be defined as simply coherent scattering and photoelectric absorption. Incoherent scattering is negligible. The complete interaction with an atom may thus be described by a complex scattered amplitude defined by an atomic scattering factor, $f_1 + if_2$, as depicted in Figs. 1 & 2. The scattered amplitude is given by this factor multiplied by that amplitude which would be scattered if the atom were replaced by a free, Thomsonian electron. Here, r_0 is the classical electron radius, m the electron mass, c the velocity of light and R the distance from the atom to the point of measurement. Because the wavelengths of interest are large as compared with the dimensions of the electron distributions within the atom, we make the important assumption here that essentially all electrons will scatter effectively in phase for all but the largest angles of scattering so that the atomic scattering factor components, f_1 and f_2 , may be considered angle independent. The complex amplitude of atomic scattering therefore will be dependent only upon the angle of scattering, 2θ , through the polarization

factor, $P(2\theta)$, of the Thomsonian term. $P(2\theta)$ is equal to unity or $\cos 2\theta$ depending upon whether the incident electric vector is perpendicular to or parallel to the plane of scattering. As will be discussed below, the relative roles of the coherent scattering and the photoelectric absorption will be expressed through f_1 and f_2 , respectively.

The relativistic quantum dispersion theory for atomic scattering and the calculation of the atomic scattering factors has been presented by Crower and Lieberman [4] and by Jensen [5] (along with their references). In Fig. 2 are shown their results including the relativistic corrections, Δf_r , to the semiclassical, usual relations for f_1 and f_2 . Here Z is the atomic number, h Planck's constant, mc^2 rest mass energy of the electron, E_{tot} the total energy of the atom and E the photon energy. Crower and Lieberman have estimated E_{tot} (a negative quantity) for all the elements and from their table we have fit the following polynomial for the larger term in Δf_r .

$$\frac{5}{3} \frac{E_{tot}}{mc^2} = 2.19 \times 10^{-4} Z^2 - 1.03 \times 10^{-4} Z^2.$$

LOW ENERGY X-RAY SCATTERING

$$E(\theta, \lambda) = -[E_0 \left(\frac{r_0}{R} \right) P(2\theta)] (f_1(\lambda) + if_2(\lambda))$$

Figure 1

THE ATOMIC SCATTERING FACTOR, $f_1 + if_2$

RELATIVISTIC QUANTUM DISPERSION RELATIONS:

$$f_2(E) = \frac{E\mu_a(E)}{(2\pi r_0 hc)} \quad \mu_a(E) \text{--ATOMIC PHOTOIONIZATION CROSS SECTION}$$

AND

$$f_1(E) = Z + \frac{1}{(\pi r_0 hc)} \int_0^{\infty} \frac{e^2 \mu_a(E') dE'}{E^2 - E'^2} + \Delta f_r,$$

$$\text{WHERE } \Delta f_r = \frac{5}{3} \frac{E_{tot}}{mc^2} - \frac{Z}{2} \left(\frac{E}{mc^2} \right)^2$$

WHICH IS NEGLIGIBLE FOR THE LOW ENERGY X-RAY REGION.

Figure 2

For the low energy x-ray region it is immediately evident that this and the second relativistic term in Δf_r are completely negligible except near thresholds where f_1 becomes small as compared with Z . An important argument here, therefore, is that for the low energy x-ray region, the atomic scattering factor, $f_1 + if_2$, can be uniquely determined through these relations in terms of the total atomic photoionization cross section and its dependence upon photon energy. It may be noted that f_2 is directly proportional to the atomic photoionization cross section for a given photon energy, E . It will exhibit the same structures near thresholds as does the photoionization cross section, $\mu(E)$. The relation for f_1 suggests that the important anomalous scattering contribution (through the integral term) depends upon a knowledge of the photoionization cross section dependence upon photon energy from a very small to very large value of photon energy. The nature of this integral, however, is that its value is sensitive to an integration range of energies relatively close to E . In our calculations [1] for f_1 , we have found it convenient to use a range from 30 eV to 85 keV with our greatest concern for knowing precisely the cross sections in the intermediate region of 100-2000 eV.

In Figs. 3, 4 and 5 we present examples of plots of the calculated scattering factor components, f_1 and f_2 , for aluminum, copper and xenon. In the f_2 plots for the photon energy region below about 300 eV we have indicated values corresponding to representative, available experimental data including that which we have adopted for this fitting. [6-10] It is important to note that throughout the low energy x-ray region, the f_1 values are appreciably different from the classical Thomsonian value of Z (as a result of electronic binding and consequent anomalous scattering).

It is proposed here that with sufficient accuracy we may assume that the low energy x-ray photoionization cross sections and, correspondingly, the atomic scattering factors are atomic-like even in the chemical and solid states. This effect is illustrated in Fig. 6 where shown is a comparison of the photoionization cross sections as measured in the vapor and in the solid state for the elements sodium, iron and barium. [11-13] Near thresholds there are characteristically large departures from the atomic-like character when the atoms are in the molecular and solid state. At the absorption edge may be sharp excitonic structures [14] and nearby may be the extended absorption fine structure (exafs) [15]. Nevertheless, as has been discussed by many authors, [16-18] above about 50 eV and away from thresholds, the photoionization cross sections are relatively independent of the state of the atomic system. In our integrations for f_1 we have used values for $\mu(E)$ that have been averaged through such structures near the thresholds.

Thus for the low energy x-ray region of interest here (100-2000 eV) we define and have tabulated the

ATOMIC SCATTERING FACTOR, $f_1 + if_2$ -- ALUMINUM

Figure 3

ATOMIC SCATTERING FACTOR, $f_1 + if_2$ -- COPPER

Figure 4

TABLE 1

$D(0.1)/D(0.25)$	1.50	1.36	1.28	1.24	1.21	1.19	1.16	1.14	1.12	1.11	1.09
$D(0.25)$	.2	.4	.6	.8	1.0	1.2	1.4	1.6	1.8	2.0	2.2

**RAR-2497 FILM CALIBRATION
FOR Al-K α (8.34 Å/1487 eV)**

Figure 6

**SENSITIVITY, S (PHOTONS/MICRON 2) $^{-1}$
VS
PHOTON ENERGY, E (eV)**

Figure 7

as the silver halide grains become more transmissive with increasing photon energy (up to the silver-L edges at about 3000 eV where the absorption efficiency of the silver halide grains is abruptly increased).

This work on the characterization of photographic emulsions appropriate for the low energy x-ray region is continuing at this laboratory on the RAR 2497 and other films including the Kodak 101-01.

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A Sensitometric Calibration of the RAR 2497 Film for the Low Energy X-Ray Region

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Described here is an operational method which has been developed for the calibration of spectroscopic films for the low energy x-ray region of 100-2000 eV, along with some preliminary photographic density, D , versus exposure, E , measurements for the RAR 2497 films. The 2497 films are the successor to the widely applied 2490 films. A comprehensive sensitometric study of the RAR 2490 has been reported by R. F. Benjamin, P. B. Lyons and R. H. Day [1]. (See also their references for a review of works on the calibration of photographic materials for this low energy x-ray region.)

Our measurements are derived directly from calibrated spectra of standard x-ray source characteristic lines as simultaneously dispersed at normal incidence along a detection circle by elliptically curved crystal/multilayer analyzers. This type of spectrograph is described elsewhere in these Proceedings [2]. The absolute peak counting rate above background is determined by a flow proportional counter that is scanned along the detection circle using a precision goniometer. Multiple exposures are then taken with the photographic films placed along the same detection circle and under identical spectrographic conditions in order to obtain the required range of values of photographic densities at the peaks of the calibrated lines. An example of the corresponding proportional counter and microdensitometer scans for several diffracted orders of the Cu-L α (13.3 A/930 eV) radiation (from an elliptically curved lead behenate analyzer--2d=120 A) is shown in Fig. 1.

For the D vs E measurements that are presented here, appropriately filtered line radiations from the following x-ray tube anodes were used: molybdenum, graphitized aluminum, anodized aluminum, copper and aluminum. These yielded the strong, easily isolated radiations: Mo-K α (64.4 A/193 eV), C-K α (44.7 A/ 277 eV), O-K α (23.6 A/525 eV), Cu-L α (13.3 A/930 eV), and Al-K α (8134 A/1487 eV). Filters were used on the x-ray tube window, on the entrance aperture (at the center of the detection circle) to the photographic film cassette [3] and on the proportional counter window. The filters for the camera and for the counter were carefully matched so that their attenuation factors cancel out in these absolute measurements. Approximately 800 A of aluminum was vacuum deposited upon the light-transparent filters to block visible and uv background light.

In order to measure the absolute photon intensity at a peak of a given spectral line, pulse height windows with a "pressure-tuned" flow proportional counter were used to eliminate high energy radiation components that might appear as high order diffraction background to the spectral line. Subatmospheric propane counter gas was used for all wavelengths longer than 10 μ . Atmospheric P-10 was used for the Al-K radiation. It is assumed that all photons of a given energy that are absorbed within the gas path of the counter will be counted and with pulse heights characteristic of that energy. The equivalence of photon absorption efficiency and photon counting efficiency was verified by measuring count rate vs counter pressure which yielded the expected pressure dependence [4].

The counter and the effective microdensitometer slit widths were matched at approximately 100 microns, which dimension is small as compared with the FWHM of the spectral lines that were measured. The photographic emulsion granularity may be considered very small at this 100 micron scale.

A Boller-Chivens Model 14213 microdensitometer was used which has continuously variable primary-illumination and objective apertures. The data presented here were microdensitometered with primary illumination of 0.1 and objective 0.25 numerical apertures. Ten neutral density filters (Balzers) of calibrated densities in the range .01 to 2.4 were used to establish the microdensitometer calibration.

The 35 mm 2497 film [5] was developed with agitation for six minutes in a film tank with full strength D-19. Standard stop bath and fixing solutions were used. Drying was at room temperature and in still air.

Figure 1

RESULTS

In Figs. 2 through 6 we present the D vs E curves for the five standard laboratory wavelengths in the 193-1487 eV photon energy region. For three of these radiations (277 eV, 525 eV and 1487 eV) we were able to compare the data with the D vs E curves as reported by Benjamin, et al [1] for the similar 2490 emulsion (light lines). It is important to note that the densities that were measured for the 2490 film were optical diffuse densities which are characteristically lower than the corresponding values as measured with an objective lens of small numerical aperture (as 0.25 which has been used in our measurements).

For the conventional microdensitometry of photographic spectra, matched numerical apertures for the illumination and the objective optics are often employed, for example, as 0.1 for low resolution, large slit operation and 0.25 for high resolution, fine slit operation. In order to permit a conversion of our D vs E data to the matched 0.1/0.1 numerical aperture measurement, we have determined by measurement on the 2497 film and presented in Table 1 the ratio $D(0.1/0.1)/$

$D(0.1/0.25)$. The decrease of the measured density values as the numerical aperture of the objective lens is increased is dependent upon the scattering power (grain size) of the particular film. These ratios can also be used to predict the equivalent optical diffuse density using the results given by Weaver [6].

In order to describe the photon energy response of the 2497 emulsion, we present in Fig. 7 the sensitivity, S , vs photon energy, E (eV). Here we have used the definition for sensitivity, S , as the reciprocal of that exposure value which yields a density of 0.5 as measured here with our 0.1/0.25 microdensitometer numerical apertures. These values for the sensitivity, S , can be used to estimate corresponding values as measured with other objective lens numerical apertures by using the data presented in Table 1 and the results presented in Ref. 6.

The sharp drop in this sensitivity curve is the result of the sudden increase in the absorption of the gelatine overcoating at the carbon-K edge (280 eV). It is expected that this sensitivity will continue to increase essentially monotonically with photon energy to about 2000 eV in which region it will begin to drop off

RAR-2497 FILM CALIBRATION
FOR Mo-M γ (64.4 Å/193 eV)

Figure 2

RAR-2497 FILM CALIBRATION
FOR O-K α (23.6 Å/525 eV)

Figure 4

RAR-2497 FILM CALIBRATION
FOR C-K α (44.7 Å/277 eV)

Figure 3

RAR-2497 FILM CALIBRATION
FOR Cu-L α (13.3 Å/930 eV)

Figure 5

ATOMIC SCATTERING FACTOR, $f_1 + if_2$ -- XENON

Figure 5

atomic scattering factors (a) as uniquely defined by the best available photoionization cross section data; (b) as being essentially independent of scattering angle; and (c) as being effectively independent of the state of the atomic system--except for photon energies near thresholds.

11. LOW ENERGY X-RAY INTERACTION DESCRIPTION

Generally one may treat such problems as the transmission of radiation, particle scattering, specular and Bragg reflection with a macroscopic description as an electromagnetic wave boundary value problem using material constants such as the dielectric constant, K , and the refractive index, n_r , or equivalently, by an atomic approach by summing the atomic scattered amplitudes from the irradiated atomic system and using the atomic scattering factors. By comparing the solutions of such interaction problems by these approaches, the following relationships between the complex dielectric constant, K , the refractive index, n_r , and the atomic scattering factors for the x-ray region are directly established.

For the low energy x-ray region, we define the complex dielectric constant, K , as

$$K = 1 - \alpha - i\gamma \quad (1)$$

and the complex refractive index, n_r , by

$$n_r = 1 - \delta - i\beta, \quad (2)$$

where characteristically these unit decrements, α , γ , δ and β , are small as compared with unity. We then find that the following relationships between the atomic and the macroscopic parameters obtain:

$$\delta = \frac{r_0 \lambda^2}{2\pi} n_f \bar{f}_1 = \frac{\alpha}{2} \quad (3)$$

$$\beta = \frac{r_0 \lambda^2}{2\pi} n_f \bar{f}_2 = \frac{\gamma}{2}, \quad (4)$$

where the average atomic scattering factor per unit volume, $n_f \bar{f}_i$, is given by

$$n_f \bar{f}_1 = \sum_q n_q f_{1q} \quad (5)$$

$$n_f \bar{f}_2 = \sum_q n_q f_{2q} \quad (6)$$

Here n_q is the number of atoms per unit volume of type- q .

Usually the E & M boundary value solutions can be more formal, rigorous and, however, more tedious and less intuitive. Often a description by summing over atomic scattered amplitudes, which is phenomenological, is also more flexible and amenable to practical approximation.

In transmission, scattering, specular and Bragg reflection description, a first step in summing the atomic scattered amplitudes over a given irradiated system of atoms is illustrated in Fig. 7. Here the amplitude that is transmitted and specularly reflected by an elementary atomic plane is described. The absorptive factor, σ , in the transmitted direction, and the reflective factor, s , for the coherent constant phase scattering geometry as allowed only in the specular direction, 2θ , may be related to the atomic scattering factor, $f_1 + if_2$, by simply integrating over equiphase fresnel zones throughout the plane [3].

If, as in many practical systems, the atomic layers are within periodic systems of layers as in planar crystals or in multilayers, with a periodicity length normal to the surface equal to d , σ and s may be simply generalized for this layer system of thickness, d , in terms of the average scattering factor per unit volume, n_f , defined in Eq. (5), and a structure factor per unit volume, $\phi f_1 + i\phi f_2$.

Upon summing over the scattered amplitudes within this layer system a composite scattering factor per unit volume for scattering in a direction 2θ is defined as

PHOTOIONIZATION CROSS SECTIONS ATOMIC VS SOLID STATE

VAPOR ———
METAL ······

Figure 6

AMPLITUDES REFLECTED AND TRANSMITTED

FOR M ATOMS / UNIT AREA OF ATOMIC SCATTERING FACTOR, $f_1 + if_2$

$$\sigma = -M_0 \lambda d \frac{f_1 + if_2}{\sin \theta} \quad \text{AND} \quad s = -M_0 \lambda d \frac{f_1 + if_2}{\sin \theta} P(2\theta)$$

FOR M UNIT CELLS / UNIT AREA OF STRUCTURE FACTOR, $F_1 + iF_2$
AND OF AVERAGE ATOMIC SCATTERING FACTOR, $\bar{f}_1 + i\bar{f}_2$

$$\sigma = -M_0 \lambda d \frac{\bar{f}_1 + i\bar{f}_2}{\sin \theta} \quad \text{AND} \quad s = -M_0 \lambda d \frac{F_1 + iF_2}{\sin \theta} P(2\theta)$$

Figure 7

the unit cell structure factor per unit volume as follows:

$$\phi F = \frac{1}{Ad} \sum_p x_p (f_{1p} + if_{2p}) e^{-\left(\frac{4\pi \sin \theta}{\lambda}\right) z_p} \quad (7)$$

where the volume of the unit cell is Ad and within the unit cell at a position z_p from a reference plane there are x_p atoms of type- p .

As is often possible, if z_p may be measured from a central symmetry plane, the ϕF_1 and ϕF_2 components may then be written simply as

$$\phi F_1 = \frac{1}{Ad} \sum_p x_p f_{1p} \cos\left(\frac{4\pi \sin \theta}{\lambda} z_p\right) \quad (8)$$

$$\phi F_2 = \frac{1}{Ad} \sum_p x_p f_{2p} \cos\left(\frac{4\pi \sin \theta}{\lambda} z_p\right) \quad (9)$$

The next step in an interaction description is to sum the wave amplitudes from a given system of planes of atoms (or of unit cells) and for a given angle of scattering, 2θ . As the initial wave, as depicted in Fig. 7, proceeds to the next layer it will be partially reflected again to contribute to the total reflected wave system and this partially reflected wave will also partially reflect back as a component to be added to the initial transmitted wave system, etc. In this way the total transmitted and reflected wave systems may contain the contributions of many such multiply reflected components. The works of Darwin and Prins were perhaps the first that present a relatively simple solution for the total reflected and transmitted wave systems. [2,3, 19,20] Their approach was to write the self-consistent, difference equations for the transmitted amplitude, T_n , and total reflected amplitude, S_n , for successive layers (indexed by n) taking into account the phase shift, $k d \sin \theta$, of the waves between layers. We refer the interested reader to the relatively simple and straightforward solution of these difference equations for the reflected wave as a function only of d , θ , σ and s . Recently Smirnov [21] has written the difference equations as differential equations for a continuous set of close-spaced planes in order to treat, in particular, the reflection of x-rays from an amorphous medium interface. Smirnov's solution for a perfectly smooth interface immediately reduces to the familiar Fresnel equations as written for x-ray reflection by simply replacing the f_1 and f_2 parameters by their optical constant

equivalents through relations (3) and (4).

This inclusion of the effects of multiple reflection and absorption is called a dynamical approach. In certain problems a simple and useful approximation for the summing for the total reflected wave system from a system of planes can be obtained by neglecting the effect of the multiple reflection and the absorption reduction of the incident wave. For example, this can be appropriate for scattering by small crystals or particle systems for which relatively few planes are involved. This simplification in the summing of the reflected waves is called a kinematical approach.

In the sections that follow, we would like to summarize the results of such calculations for some examples of practical interest.

A. NORMAL INCIDENCE TRANSMISSION OF LOW ENERGY X-RAYS

Using the Darwin-Prins-Smirnov (DPS) approach, we have calculated the total transmitted and reflected amplitude for a normally incident, unpolarized plane wave of x-rays for uniform, amorphous solid. Taking the square of the moduli of these amplitudes, we find that the reflected intensity is negligibly small, as expected, and that the transmitted intensity is reduced exponentially with distance z from the surface as $\exp(-2r_0 n \bar{f}_2 z)$, where $n \bar{f}_2$ is the average scattering factor component, f_2 , per unit volume as given by Eq. (5). From an E & M, boundary value solution for the Poynting vector describing this transmitted energy flow, we find [17] that it is reduced with z by the factor $\exp(-4\pi \bar{f}_2 / \lambda z)$. Comparing these exponential factors with that defined in terms of the linear absorption coefficient, μ_2 , we obtain the relations

$$\mu_2 = \frac{4\pi \bar{f}_2}{\lambda} = 2r_0 n \bar{f}_2 \quad (10)$$

which is consistent with relation (4). This result may also be written as

$$\bar{f}_2 = \frac{E_{\mu_2}(E)}{2\pi r_0 h c} \quad (11)$$

where μ_2 is an atomic (or molecular) photoionization cross section equal to μ_2/n . This result also follows from the quantum theory of dispersion as noted in Fig. 2.

B. THE QUANTUM YIELD FOR LOW ENERGY X-RAY PHOTOCATHODES

In a recent work [23] we have shown experimentally and by a simple phenomenological model that the number of electrons that are photoemitted per normally incident photon, the quantum yield, γ , is dependent upon photon energy through the factor, $\rho \mu(E)$ or $E \mu_2(E)$. E is the photon energy, ρ , the mass density of the photocathode, μ and μ_2 are the mass and linear photoionization cross sections, respectively. We may thus write for the photocathode efficiency

$$\gamma \sim n \bar{f}_2 \quad (12)$$

by applying Eq. (11) where $n \bar{f}_2$ is the average scattering factor, f_2 , per unit volume for the photocathode and given in Eq. (5). Thus the f_2 parameters which have tabulated here and in Ref. 1 can be used directly to estimate the photon energy dependence of x-ray photocathodes.

C. SMALL ANGLE SCATTERING OF LOW ENERGY X-RAYS

As has been noted in Sec. II-A, a measurement of the attenuation of the transmitted intensity through a uniform, homogeneous material can be used to determine the photoionization cross section, μ , and the atomic scattering factor component, f_2 . If the sample material consists of small particles or voids of dimensions large compared with the wavelength of the incident radiation, the direct beam will be reduced further by the resulting coherent scattering. In order to estimate this effect

and/or to evaluate material scattering generally, a description of the scattering by spherical particles or voids is presented here as a relevant example.

This problem has been discussed in some detail in a previous work by the author [24]. By neglecting absorption within the sphere (each differential plane receiving essentially the same incident intensity) and neglecting multiple interference, we may calculate, relatively easily, the scattered intensity distribution by a kinematical approach. Integrating the differential amplitudes which are proportional to the circular section area of $\pi(R^2 - z^2)$ (see Fig. 8) and with phase angle relative to that for the central plane, $4\pi z \sin \theta / \lambda$, (with 2θ the angle of scattering) we obtain the total amplitude of the scattered wave [24]. Taking the modulus squared, we then obtain the intensity distribution at a distance, r , from a spherical particle.

$$I = I_0 \left(\frac{4\pi^2 R^2}{r^2} \right) \left((n_f^2)^2 + (n_g^2)^2 (1 + \cos^2 2\theta) \right) \left(\frac{J_{3/2}(u)}{u} \right)^2. \quad (13)$$

Here again n_f^2 and n_g^2 are the averaged scattering factor components per unit volume, from Eq. (5); $u = \frac{4R \sin \theta}{\lambda}$, and $J_{3/2}(u)$ is the Bessel function of order $3/2$. For small angle scattering, i.e., for $\lambda \ll R$, the central maximum is well approximated by a Gaussian distribution

$$I = \frac{8\pi^2}{9} \frac{R^6 r^2}{r^2} \left((n_f^2)^2 + (n_g^2)^2 (1 + \cos^2 2\theta) \right) I_0 e^{-\frac{u^2}{5}} \quad (14)$$

of angular width, $\Delta \theta = \sqrt{5/8} \lambda / R$.

The E & M boundary value solution was rigorously obtained in series form using Legendre polynomials by Mie [25]. This solution was expressed in closed form by Hart and Montroll [26] and by van de Hulst [27] for "soft" spheres for which absorption was not completely neglected. We have taken this dynamical model result which may be appropriate for the lower energy x-ray region and have shown that it reduces to Eq. (13) in the low absorption limit by again replacing the optical constants, δ and β , by the equivalent functions in f_1 and f_2 given in Eqs. (3) and (4). [24] By integrating over a sphere to obtain the total scattering through all angles we have obtained expressions for the total cross sections. The total cross section per particle, s_p , and the total cross section per gram, s_m , as derived from Eq. (13), become

$$s_p = r_0^2 \lambda^2 R^6 \left((n_f^2)^2 + (n_g^2)^2 \right) \\ s_m = \frac{3}{4\pi} \frac{R^2 \lambda^2}{\rho_0} \left((n_f^2)^2 + (n_g^2)^2 \right) \quad (15)$$

(ρ_0 is the mass density of the particle.)

If the scattering medium consists of spherical particles of an average atomic scattering factor per unit volume, $n'(\bar{f}_1' + i\bar{f}_2')$ imbedded in a material of that equal to $n(\bar{f}_1 + i\bar{f}_2)$, it can be shown that the kinematical result, Eq. (13), will obtain if we simply replace n_f and n_g by the difference parameters, $(n_f - n'f_1')$ and $(n_g - n'f_2')$. For voids, $f_1' = f_2' = 0$.

If the transmission sample is sufficiently thick so that multiple scattering is significant, the angular distribution of the intensity is broadened over that predicted by Eq. (13). This effect is discussed in Ref. [24].

D. SPECULAR REFLECTION BY X-RAY MIRRORS

As noted above, Smirnov [21] has expressed the Darwin-Prins difference equations as differential equations descriptive of the reflection and transmission for a continuous set of planes with spacing between the atomic reflecting planes that is small as compared with the wavelength. (He describes this case as the zero-order Bragg reflection.) After deriving the expression for total reflection from a perfectly smooth interface that reduced immediately to that predicted through the

LOW ENERGY X-RAY PARTICLE SCATTERING

LOW ANGLE SCATTERING CROSS SECTION/PARTICLE

$$s_p = \phi^2 R^6 \frac{2}{3} \lambda^2 (f_1^2 + f_2^2)$$

(ϕ = ATOMS/UNIT VOLUME)

Figure 8

Fresnel equations (E & M boundary value solution), Smirnov et al. [28] then extended these calculations to predict the effect of surface roughness upon x-ray mirror reflection and thus explain thin often observed departures of some experimental curves from the Fresnel curves.

For the low energy x-ray region, it is important not to assume that the specular reflection occurs only for the small glancing angles as is usually assumed. [2, 3, 21, 28] In order to obtain a precise large angle solution for the reflection of low energy x-rays, the author [22] has specialized the rigorous and general solutions of Mahan [29] for the reflection of a plane electromagnetic wave from a semi-infinite homogeneous, absorbing medium. We have shown in that solution that for the x-ray region, the reflection equation can be expressed completely in terms of a complex dielectric constant given by

$$K = 1 - (1 - \epsilon) - \frac{i2\sigma}{\nu} = 1 - \alpha - i\gamma \quad (16)$$

(using here only, Mahan's notation). ϵ is the dielectric constant, σ the conductivity constant and ν the radiation frequency.

This dielectric constant may be derived from the dipole moment per unit volume within the medium through the usual relation

$$K = 1 + \frac{4\pi M}{E}$$

where E is the electric incident field. And this dipole moment per unit volume, M , can be expressed as a sum of the atomic dipole moments which are proportional to the atomic scattering factors. We can thus derive

$$\alpha = \frac{r_0 \lambda^2}{\pi} n_f^2 \\ \gamma = \frac{r_0 \lambda^2}{\pi} n_g^2 \quad (17)$$

which relations also follow from Eqs. (1) through (4) (deduced by comparing the E & M and atomic scattering solutions).

We may now write Mahan's reflection intensity as specialized for large angle, low energy x-ray reflection as a function of a convenient parameter, ρ , defined by

$$\rho^2 = \frac{1}{2} (\sin^2 \theta - \alpha + \sqrt{(\sin^2 \theta - \alpha)^2 + \gamma^2}). \quad (18)$$

Here θ is the grazing incidence angle and α and γ are given by f_1 and f_2 through Eq. (17). (For small θ , α and γ , the parameter, ρ , becomes equal to the internal angle that the refracted beam makes with the reflecting surface.)

We define I_p and I_0 as the ratios of the reflected intensity to the incident intensity for the polarized components with the E-vector perpendicular to and

BERYLLIUM MIRROR REFLECTIVITY

Figure 9

parallel to the plane of reflection respectively. We may then write

$$I_o(\theta) = \frac{4\rho^2(\sin\theta - \rho)^2 + \gamma^2}{4\rho^2(\sin\theta + \rho)^2 + \gamma^2} \quad (19)$$

and for the polarization ratio

$$\frac{I_p(\theta)}{I_o(\theta)} = \frac{4\rho^2(\rho - \cos\theta\cot\theta)^2 + \gamma^2}{4\rho^2(\rho + \cos\theta\cot\theta)^2 + \gamma^2} \quad (20)$$

and finally for the total reflected intensity for an unpolarized incident beam

$$I(\theta) = \frac{1}{2}I_o(1 + I_p/I_o). \quad (21)$$

We have shown from Mahan's exact solution that the absorption factor in the Poynting vector that describes the energy flow of low energy x-rays into the medium is equal to $\exp(-2\pi\gamma z/\lambda\rho)$ where z is the penetration depth as measured normally to the reflecting surface. We may therefore define a $1/e$ depth involved in x-ray reflection by the relation

$$d_{1/e} = \frac{\lambda\rho}{4\pi\gamma} \quad (22)$$

In Ref. [1] we have applied this description of the reflection of low energy x-rays from perfectly smooth interfaces to establish detailed tables in photon energy and reflection angle for the mirrors beryllium, carbon, aluminum oxide, aluminum, fused quartz, nickel, copper and gold. As examples of such calculations we present here in Figs. 9 and 10 the reflectivity curves for beryllium and for nickel. In a companion paper of these proceedings, we also present the reflectivity-vs- θ curves for those characteristic long wavelengths for which we could also include reported experimental points for comparison.

D. BRAGG REFLECTION FROM MULTILAYERS AND CRYSTALS

Using the elementary interaction as described in Fig. 7 for a plane wave reflecting and transmitting at a single layer of unit cell structures, Compton and Allison have followed a Darwin-Prins approach to proceed to write equations for the total transmitted and reflected waves that obtain for any arbitrary, successive set of planes within a crystal of an infinite number of planes and of spacing equal to d . These difference equations were then solved with the following important results.

We define the incident amplitude of the plane wave as T_0 and the total reflected wave amplitude leaving the surface as S_0 . It is shown that the total transmitted wave proceeding into the crystal that reaches the N th layer (including the contributions of all possible multiple reflections) may be given simply by

$$T_N = T_0 x^N, \quad (23)$$

where the attenuation factor per layer, x , is assumed to

NICKEL MIRROR REFLECTIVITY

Figure 10

be only slightly less than unity and thus we may define x here by

$$x = (-1)^m e^{-\eta}, \quad (24)$$

where m is the order of diffraction and

$$\eta = \sqrt{s^2 - (\sigma + \xi)^2} \quad (25)$$

and

$$\xi = \frac{2\pi}{\lambda} d(\sin\theta - \sin\theta_0) \quad (26)$$

(θ_0 is defined by the Bragg relation, $m\lambda = 2d\sin\theta_0$.) In Eq. (25) we choose the plus or minus sign so that the real part of η will have the (physically significant) positive value. It also follows as suggested in Fig. 11 that the total wave amplitude at the N th layer that is proceeding upward in the Bragg reflected direction (including all multiple interference contributions) may be written as

$$S_N = S_0 x^N. \quad (27)$$

The solution of the self-consistent difference equations for the ratios of the total reflected to incident amplitudes at the crystal surface and at the N th layer are given by

$$\frac{S_0}{T_0} = \frac{-s}{(\sigma + \xi) + \sqrt{(\sigma + \xi)^2 - s^2}} = \frac{S_N}{T_N}. \quad (28)$$

Finally, by taking the modulus squared of the amplitude ratio as a function of the angle, θ , here in terms of the atomic scattering factors,

$$I_{\omega}(\theta) = \left| \frac{-s}{(\sigma + \xi) + \sqrt{(\sigma + \xi)^2 - s^2}} \right|^2 \quad (29)$$

We would like now to apply this Darwin-Prins approach (difference equation solution for small values of σ and s) as outlined above in order to estimate the effect of limiting the crystal or multilayer to a finite number of layers, N . We suggest that the total amplitude of reflection for this finite system should be

N-DEPENDENT DARWIN-PRINS MODEL

Figure 11

that reflected for the infinite-layer system minus that total wave amplitude reflected from the multilayer system from $N+1$ to ∞ . Because S_0/T_0 and S_N/T_N both describe the amplitude ratios from a surface above an infinite number of layers, these must be equal. And because S_N must also be attenuated by the same factor, X^N for its value at the surface, we then obtain (as presented in Fig. 11) the amplitude ratio for the first N layers as follows:

$$\left(\frac{S_0 - S_0 x^{2N}}{T_0} \right) = \frac{S_0}{T_0} (1 - x^{2N}). \quad (30)$$

Finally we may write for a modified Darwin-Prins expression for a finite number of layers, N^*

$$I_N(\theta) = I_{\infty} \{ (1 - e^{-2N\eta}) \}^2. \quad (31)$$

Because, for practical crystal systems, the intensities are significantly large only at angle, θ , near the diffraction peak, we may, with good approximation, rewrite the expressions for the structure factor per unit volume to be used in calculating these reflection intensities and as given in Eqs. (8) and (9) with θ set equal to the Bragg angle, θ_0 defined by $m\lambda = 2d \sin \theta_0$. These become

$$\phi_{F1} = \frac{1}{Ad} \sum_p x p f_{1p} \cos \frac{2\pi m z p}{d} \quad (32)$$

and

$$\phi_{F2} = \frac{1}{Ad} \sum_p x p f_{2p} \cos \frac{2\pi m z p}{d}. \quad (33)$$

For the sputtered/evaporated multilayer systems consisting of successive double layers of thickness, d , with a "heavy" layer of thickness $1d$ and scattering factor per unit volume, $n(f_1 + if_2)$ and a "light" layer of thickness $1 - 1d$ and of scattering factor per unit volume $n'(f_1' + if_2')$ we obtain from an integral equivalent of Eqs. (32) and (33) for such a system of continuous layers the following for the structure factor per unit volume.

$$\phi_{F1} = \frac{1}{m\pi} (n f_1 - n' f_1') \sin \frac{1}{2} m \pi. \quad (34)$$

and

COMPARISON OF MULTILAYER MODEL CALCULATIONS

CHARACTERISTIC MATRIX APPROACH (E & M BOUNDARY VALUES) -- LEE (1981)

MODIFIED DARWIN-PRINS -- LEE (1981)

MODIFIED DARWIN-PRINS -- HENKE (1981)

Figure 12

EFFECTS OF INTERFACE DIFFUSION

UPON THE STRUCTURE FACTOR/UNIT VOLUME -- $\phi_{F1} + i\phi_{F2}$
AND THE ATOMIC SCATTERING FACTOR/UNIT VOLUME, $n f_1 + i n f_2$

— SHARPLY DEFINED INTERFACE —

$$\phi_{F1} = \frac{n f_1 - n' f_1'}{\pi}$$

$$\phi_{F2} = \frac{n f_2 - n' f_2'}{\pi}$$

$\phi_{F1} = \phi_{F2} = 0$ FOR EVEN ORDERS ONLY

— SINUSOIDALLY DIFFUSED INTERFACE —

$$\phi_{F1} = \frac{n f_1 - n' f_1'}{4}$$

$$\phi_{F2} = \frac{n f_2 - n' f_2'}{4}$$

$\phi_{F1} = \phi_{F2} = 0$ FOR ALL HIGH ORDERS

Figure 13

$$\phi_{F2} = \frac{1}{m\pi} (n f_2 - n' f_2') \sin \frac{1}{2} m \pi. \quad (35)$$

Lee [30] has recently reported an E & M boundary value solution for the periodic multilayer system as defined above using a characteristic matrix approach (CMA-Lee). He has shown that this rigorous solution for the intensity distribution at a diffraction peak will reduce to the Darwin-Prins expression for I_{∞} , and that another relatively simple modified form of the Darwin-Prins equation can be written with a correction term that introduces a dependence upon a finite number of layers, N . These results have also been discussed in Ref. [1].

It is of interest to compare reflectivity curves for multilayer systems as predicted by the modified Darwin-Prins expression given in Eq. (31) (DP-Henke) with the rigorous result (CMA-Lee) and its reduced version (DP-Lee). These comparisons are presented in Fig. 12. These were calculated for the reflection of $0-K\alpha$ (23.6 Å/525 eV) radiation from a tungsten/carbon multilayer of $2d = 40$ Å, $r = 0.3$ and for N equal to 30 and 100. It is interesting to note that the three descriptions yield essentially the same diffraction line widths and the modified Darwin-Prins expressions give somewhat higher peak values and consequently slightly higher integrated reflectivities.

As noted earlier, Smirnov et al. [28] have found the Darwin-Prins approach to be very effective in an analysis for the effects of surface roughness in x-ray reflection. They have shown that the same effects can be produced by a suitably chosen graded density interface as by a given surface roughness structure. It is suggested here that the sputtered/evaporated multilayer systems such as tungsten/carbon may exhibit changes in their reflectivity characteristics which can be explained either by interface roughness or equivalently by a graded tungsten carbide interface. For example, some of the tungsten/carbon multilayer systems which we have characterized spectroscopically have yielded essentially no high-order reflections for what were

COMPARISON OF CALCULATED & EXPERIMENTAL FOR INTEGRATED REFLECTIVITY, R, AND ENERGY RESOLUTION, ΔE

TUNGSTEN/CARBON MULTILAYER, $2d=44.2$ Å, $N=62$, $\Gamma=0.5$

CALCULATED--(1) SHARPLY DEFINED AND
(2) DIFFUSED INTERFACES

EXPERIMENTAL • HENKE, et al. (1980)

Figure 14

fabricated as $\Gamma = 0.5$ multilayers. As may be noted from Eqs. (34) and (35), such multilayers should have zero intensity even-order reflections only if the interfaces are sharply defined. However, if we assume that the scattering factor per unit volume with the double layer varies sinusoidally, we calculate by integration a structure factor per unit volume that is of zero value for all high order reflections. In Fig. 13 these structure factors per unit volume for the sharply defined multilayer and for the corresponding diffused multilayer are presented. In Fig. 14 we show the calculated integrated reflectivities (R) and the diffraction line widths (ΔE) using the modified Darwin-Prins expression with ϕF values for the two types of interface and compare these with our experimental data for the same multilayer system.

Many practical crystal and multilayer systems may also have a mosaic structure (illustrated schematically in Fig. 15) consisting of small crystal segments which, however, are usually large as compared with the wavelengths involved, and the normals to each crystal segment face have a random, small angle distribution about an average normal to the macroscopic total crystal surface. The width of the associated rocking curve, $1(\theta)$, from such a mosaic crystal is thereby increased by this angular distribution width which is usually not predictable. Nevertheless, the total area under the rocking curve, i.e., the integrated reflectivity, is not dependent upon the degree of mosaic alignment and can be simply calculated using a kinematical model. This is because one may usually assume that the crystal segment thickness is such that each atomic plane receives essentially the same incident intensity (negligible absorption within the crystallite). Summing over the differential amplitudes for the small crystal to obtain the amplitude of reflection and then squaring to obtain the intensity of reflection per crystal segment, adding

Figure 15

these intensities over the mosaic collection (assuming their amplitudes are in random phase) and finally integrating over angles the integrated reflectivity for a mosaic crystal, R_m , is obtained [2,3] which may be written as

$$R_m = \frac{r_0^2 h^2 [(\phi F_1)^2 + (\phi F_2)^2]}{16\pi B} [1 - \exp(-\frac{2\mu t}{\sin \theta_0})] \times \frac{1 + \cos^2 2\theta_0}{\sin^2 \theta_0} \quad (36)$$

where, for a finite mosaic crystal, μ , ρ and t are the mass photoionization cross section, the average density and the thickness, respectively.

In Ref. [1] we have presented detailed tables and plots characterizing five examples each of the three important, practical analyzer systems that are effective in low energy x-ray spectroscopy, viz., the sputtered/evaporated multilayers, the molecular multilayers (Langmuir-Blodgett type) and the acid phthalate crystals. Presented here in Figs. 16, 17 and 18 are examples of such calculations using the methods and the atomic scattering factors as described here. The calculated characteristics for the tungsten/carbon multilayer, the lead myristate molecular multilayer and the thallium acid phthalate crystal plotted here are the integrated reflectivities, R , in milliradians (mosaic) and R_p (by integrating under the modified Darwin-Prins rocking curve), the percent reflectivity, $P(\%)$, at the diffraction peak, the full-width-at-half-maximum of the rocking curve in eV, and the resolving power $E/\Delta E$.

Finally it is of considerable current interest in x-ray optics development to determine the characteristics of Bragg reflection from multilayers and crystals at near normal incidence (for example, for possible applications in x-ray interferometers, for end "mirrors" in x-ray laser cavities, or for reflective coatings for normal incidence mirror optics for x-ray telescopes and microscopes). At near-normal incidence, the width of the diffraction pattern for a given wavelength becomes appreciably broadened and it is important not to approximate ξ as given exact in Eq. (26) in terms of the difference angle, $\theta - \theta_0$, as is usually done in x-ray Bragg reflection descriptions. [2,3] If the diffraction width is appreciably broadened, it may be important not to use the approximate expressions (32) and (33) for the structure factor components but rather the exact expressions (8) and (9). It may not be sufficiently accurate to discard terms of higher order than ξ^2 in either the characteristic matrix approach [30] or in the Darwin-Prins approach.

As an example of a normal incidence calculation, we have calculated the rocking curve at about $\theta = 90^\circ$ for a multilayer of tungsten/carbon of $\Gamma = 0.4$. The $2d$ values were obtained for each of five wavelengths in the low energy x-ray region by maximizing the respective intensities for 90° incidence. We have used the CMA model relation of Lee [30] for these calculations and have plotted the diffraction curve for O-K α (23.6 Å/525 eV) and have compared the wavelengths with the optimized $2d$ -values in Fig. 19.

III. CONCLUSIONS--SOME COMPARISONS WITH EXPERIMENT

The predictions of the characteristics of Bragg reflection from multilayers and crystals are usually very sensitive to the appropriateness of the models that are adopted and to the atomic scattering factor data that is used. The experimental characterization of these systems can thus be an important test of the methods and of the atomic scattering factor data that have been presented here.

At this time, it is not possible to define accurately the detailed structure of the "synthetic crystals" such as the sputtered/evaporated and the molecular multilayers as we might crystallographically

TUNGSTEN-CARBON MULTILAYER

$2d = 40 \text{ \AA}$ $\Gamma = 0.4$ $N = 100$

Figure 16

NORMAL INCIDENCE REFLECTIVITY -- 23.6 A

TUNGSTEN/CARBON MULTILAYER $\Gamma = 0.4$ $N = 100$

Figure 19

λ	OPTIMIZED 2d - VALUE	% REFLECTION AT 90° CMA-LEE	DP-LEE
64.37	64.99	17.2	18.6
44.7	44.83	21.9	23.0
23.62	23.67	7.96	8.11
13.34	13.35	2.59	2.63
8.34	8.34	0.385	0.396

LEAD MYRISTATE

$N = 100$

$2d = 80 \text{ \AA}$

Figure 17

THALLIUM ACID PHTHALATE

$2d = 25.90 \text{ \AA}$

Figure 18

for the acid phthalate crystals, for example. Nevertheless, within the limits of experimental uncertainty, we feel that the agreement of the present experimental data with the calculations that have been described here has been generally very good.

In Fig. 14 we have presented a comparison of the measured values for the integrated reflection from a tungsten/carbon multilayer system. Here we have addressed the question as to the effect of a possible interface roughness or, equivalently, a graded tungsten carbide diffused interface upon the integrated reflectivity (for which the experimental values invariably fall somewhat below predicted values for the sputtered/evaporated systems). In Figs. 20 and 21 we present the integrated reflectivities vs photon energy for the molecular multilayer, lead myristate, and for the potassium acid phthalate crystal as calculated by the mosaic model and by the modified Darwin-Prins model. We compare these theoretical curves with our experimental values.

It is very important to note here, in Fig. 21, that the measured integrated reflectivity curve near the oxygen-K absorption edge (Blake et al.[31]) reveals a very sharp "spike" in the reflection at about 532 eV. This is a rather dramatic example of threshold structure that cannot be predicted with the calculated scattering factor data as has been discussed in Sec. 1. Such effects may need to be explained on the basis of a detailed consideration of the electronic states of the crystal including excitonic. Presented elsewhere in these proceedings by R. L. Blake will be a complete description of the excellent measurements of this threshold resonance reflection effect.

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Figure 20

Figure 21

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*Note Added in Proof: For small N , the reflected amplitude and intensity given by Eqs. (30) and (31) depart somewhat from these quantities as given by an exact description of a finite multilayer or crystal, but only in the region near the center of the diffraction peak. This is illustrated by the "squiggle" at the peak for the 30 layer system shown in Fig. 12. For a relatively large number of layers, N , as given by Eq. (31) is in good agreement with that predicted by the CMA approach as illustrated in Fig. 12 for the 100 layer system. Our approximation in deriving Eq. (31) was to use for the attenuation of a transmitted beam through N layers the quantity x^N in which x was deduced for a system of an infinite number of layers. This is, x included the interaction by multiple interference of the first N layers with the layers $N+1, \dots, \infty$. A. Rosenbluth, in a private communication, has verified this fact by showing that the more exact I_N expressions (given by Eq. (9) of the Rosenbluth and Forsyth paper of these Proceedings, and by Eq. (16) of Lee [30]) does become essentially equal to that given here in Eq. (31) for the wings of the diffraction peak and, for large N , at the center of the peak as well.

Appendix: The Atomic Scattering Factor, $f_1 + if_2$, for 94 Elements and for the 100 to 2000 eV Photon Energy Region

B. L. Henke, P. Lee, T. J. Tanaka, R. L. Shimabukuro and B. K. Fujikawa

University of Hawaii, Department of Physics and Astronomy, Honolulu, Hawaii 96822

In a recent work,¹ a "state of the art" compilation and fitting of the best available experimental and theoretical photoionization cross sections has been presented for the 30 to 10,000 eV region. Using the quantum dispersion theory, the atomic scattering factors were then uniquely determined from the photoionization cross section data for the low energy x-rays. In Ref. 1, the original data were given at fifty laboratory wavelengths along with compilation references and a description of the fitting procedures. Presented here are the f_1 and f_2 values which have been interpolated at regular intervals.

As discussed in the review papers of these Proceedings by Henke, the f_1 and f_2 parameters may be applied to calculate the low energy x-ray interactions--absorption, scattering, specular and Bragg reflection.

The corresponding value for the photoionization cross section is related to f_2 by $\sigma_{\text{PI}}(E) = Kf_2$, where K for a given element is presented at the end of each $f_1 - f_2$ table in keV-cm²/gram units. For $\sigma_{\text{PI}}(E)$ in eV-barns/atom units, K is equal to 6.987×10^7 for all atoms.

The tables are presented here at 125 values of photon energy, E (eV) and wavelength, λ (Å) with logarithmically spaced intervals by truncating to the nearest electron volt the energy as given by

$$E = 100 \times 10^{(N \log 20)/124} \text{ eV.}$$

This expression may be used for convenient computer calculation and plotting of functions of f_1 and f_2 as indexed here by N . (f_1 and f_2 have been precisely interpolated for the truncated E values as listed in these tables.) The approximate K , L and M absorption edge positions are identified within the tables.

¹"Low Energy X-Ray Interaction Coefficients: Photoionization, Scattering and Reflection," B. L. Henke, P. Lee, T. J. Tanaka, R. L. Shimabukuro and B. K. Fujikawa, Atomic Data and Nuclear Data Tables 27, No. 1 (1982).

N	E(eV)	H (1) Hydrogen		He (2) Helium		Li (3) Lithium		Be (4) Beryllium		$\lambda(A)$
		f_1	f_2	f_1	f_2	f_1	f_2	f_1	f_2	
65	480	1.00	8.84-04	2.04	2.75-02	3.16	1.66-01	4.31	5.19-01	25.83
66	492	1.00	8.36-04	2.04	2.61-02	3.15	1.58-01	4.30	4.96-01	25.20
67	504	1.00	7.91-04	2.04	2.48-02	3.15	1.51-01	4.30	4.75-01	24.60
68	516	1.00	7.50-04	2.04	2.36-02	3.14	1.44-01	4.29	4.55-01	24.03
69	529	1.00	7.08-04	2.03	2.24-02	3.14	1.37-01	4.29	4.35-01	23.44
70	542	1.00	6.70-04	2.03	2.12-02	3.14	1.30-01	4.28	4.16-01	22.87
71	555	1.00	6.35-04	2.03	2.02-02	3.13	1.24-01	4.27	3.99-01	22.34
72	569	1.00	6.00-04	2.03	1.91-02	3.13	1.18-01	4.27	3.81-01	21.79
73	583	1.00	5.68-04	2.03	1.81-02	3.12	1.12-01	4.26	3.64-01	21.27
74	597	1.00	5.38-04	2.03	1.72-02	3.12	1.07-01	4.26	3.48-01	20.77
75	612	1.00	5.08-04	2.03	1.63-02	3.12	1.02-01	4.25	3.32-01	20.26
76	627	1.00	4.81-04	2.03	1.55-02	3.11	9.71-02	4.24	3.18-01	19.77
77	642	1.00	4.55-04	2.03	1.47-02	3.11	9.24-02	4.24	3.04-01	19.31
78	658	1.00	4.30-04	2.02	1.38-02	3.11	8.75-02	4.23	2.89-01	18.84
79	674	1.00	4.06-04	2.02	1.31-02	3.10	8.29-02	4.23	2.75-01	18.39
80	690	1.00	3.85-04	2.02	1.24-02	3.10	7.93-02	4.22	2.64-01	17.97
81	707	1.00	3.64-04	2.02	1.19-02	3.10	7.58-02	4.21	2.53-01	17.54
82	725	1.00	3.43-04	2.02	1.12-02	3.09	7.19-02	4.21	2.41-01	17.10
83	742	1.00	3.25-04	2.02	1.07-02	3.09	6.86-02	4.20	2.30-01	16.71
84	760	1.00	3.07-04	2.02	1.01-02	3.09	6.52-02	4.20	2.20-01	16.31
85	779	1.00	2.90-04	2.02	9.60-03	3.08	6.20-02	4.19	2.09-01	15.92
86	798	1.00	2.74-04	2.02	9.10-03	3.08	5.89-02	4.19	2.00-01	15.54
87	818	1.00	2.59-04	2.02	8.62-03	3.08	5.60-02	4.18	1.90-01	15.16
88	838	1.00	2.45-04	2.02	8.17-03	3.07	5.32-02	4.18	1.81-01	14.79
89	858	1.00	2.32-04	2.02	7.76-03	3.07	5.07-02	4.17	1.73-01	14.45
90	879	1.00	2.19-04	2.02	7.37-03	3.07	4.82-02	4.17	1.65-01	14.10
91	901	1.00	2.07-04	2.01	6.99-03	3.07	4.58-02	4.16	1.58-01	13.76
92	923	1.00	1.96-04	2.01	6.64-03	3.06	4.35-02	4.16	1.50-01	13.43
93	945	1.00	1.85-04	2.01	6.32-03	3.06	4.14-02	4.15	1.44-01	13.12
94	968	1.00	1.75-04	2.01	6.00-03	3.06	3.94-02	4.15	1.37-01	12.81
95	992	1.00	1.66-04	2.01	5.70-03	3.06	3.74-02	4.14	1.30-01	12.50
96	1016	1.00	1.57-04	2.01	5.42-03	3.06	3.56-02	4.14	1.24-01	12.20
97	1041	1.00	1.48-04	2.01	5.13-03	3.05	3.38-02	4.13	1.18-01	11.91
98	1067	1.00	1.40-04	2.01	4.86-03	3.05	3.21-02	4.13	1.12-01	11.62
99	1093	1.00	1.32-04	2.01	4.61-03	3.05	3.05-02	4.12	1.07-01	11.34
100	1119	1.00	1.25-04	2.01	4.38-03	3.05	2.91-02	4.12	1.02-01	11.08
101	1147	1.00	1.18-04	2.01	4.15-03	3.05	2.76-02	4.12	9.69-02	10.81
102	1175	1.00	1.12-04	2.01	3.93-03	3.05	2.62-02	4.11	9.22-02	10.55
103	1204	1.00	1.06-04	2.01	3.73-03	3.04	2.49-02	4.11	8.77-02	10.30
104	1233	1.00	9.98-05	2.01	3.54-03	3.04	2.37-02	4.11	8.35-02	10.06
105	1263	1.00	9.43-05	2.01	3.36-03	3.04	2.25-02	4.10	7.95-02	9.82
106	1294	1.00	8.91-05	2.01	3.19-03	3.04	2.14-02	4.10	7.56-02	9.58
107	1326	1.00	8.41-05	2.01	3.03-03	3.04	2.03-02	4.10	7.19-02	9.35
108	1358	1.00	7.95-05	2.01	2.88-03	3.04	1.93-02	4.09	6.85-02	9.13
109	1392	1.00	7.50-05	2.01	2.73-03	3.03	1.83-02	4.09	6.51-02	8.91
110	1426	1.00	7.08-05	2.01	2.60-03	3.03	1.74-02	4.09	6.20-02	8.69
111	1460	1.00	6.70-05	2.01	2.47-03	3.03	1.65-02	4.08	5.91-02	8.49
112	1496	1.00	6.32-05	2.01	2.34-03	3.03	1.57-02	4.08	5.62-02	8.29
113	1533	1.00	5.97-05	2.01	2.21-03	3.03	1.48-02	4.08	5.34-02	8.09
114	1570	1.00	5.64-05	2.01	2.10-03	3.03	1.41-02	4.07	5.08-02	7.90
115	1609	1.00	5.32-05	2.01	1.97-03	3.03	1.34-02	4.07	4.83-02	7.71
116	1648	1.00	5.03-05	2.01	1.88-03	3.03	1.27-02	4.07	4.59-02	7.52
117	1688	1.00	4.76-05	2.01	1.78-03	3.03	1.20-02	4.07	4.37-02	7.34
118	1730	1.00	4.49-05	2.00	1.68-03	3.02	1.14-02	4.06	4.15-02	7.17
119	1772	1.00	4.24-05	2.00	1.59-03	3.02	1.08-02	4.06	3.95-02	7.00
120	1815	1.00	4.01-05	2.00	1.50-03	3.02	1.02-02	4.06	3.75-02	6.83
121	1860	1.00	3.78-05	2.00	1.41-03	3.02	9.70-03	4.06	3.56-02	6.67
122	1905	1.00	3.57-05	2.00	1.34-03	3.02	9.20-03	4.06	3.38-02	6.51
123	1952	1.00	3.37-05	2.00	1.26-03	3.02	8.71-03	4.05	3.21-02	6.35
124	2000	1.00	3.18-05	2.00	1.19-03	3.02	8.25-03	4.05	3.05-02	6.20

$E_H(E)$
 f_1

41725

10507

6059.

4667.

$keV\text{-cm}^2$
gram

Atomic
Weight

1.008

4.003

6.941

9.012

amu

N	E(eV)	H (1) Hydrogen		He (2) Helium		Li (3) Lithium		Be (4) Beryllium		$\lambda(\text{\AA})$
		f_1	f_2	f_1	f_2	f_1	f_2	f_1	f_2	
65	480	1.00	8.84-04	2.04	2.75-02	3.16	1.66-01	4.31	5.19-01	25.83
66	492	1.00	8.36-04	2.04	2.61-02	3.15	1.58-01	4.30	4.96-01	25.20
67	504	1.00	7.91-04	2.04	2.48-02	3.15	1.51-01	4.30	4.75-01	24.60
68	516	1.00	7.50-04	2.04	2.36-02	3.14	1.44-01	4.29	4.55-01	24.03
69	529	1.00	7.08-04	2.03	2.24-02	3.14	1.37-01	4.29	4.35-01	23.44
70	542	1.00	6.70-04	2.03	2.12-02	3.14	1.30-01	4.28	4.16-01	22.87
71	555	1.00	6.35-04	2.03	2.02-02	3.13	1.24-01	4.27	3.99-01	22.34
72	569	1.00	6.00-04	2.03	1.91-02	3.13	1.18-01	4.27	3.81-01	21.79
73	583	1.00	5.68-04	2.03	1.81-02	3.12	1.12-01	4.26	3.64-01	21.27
74	597	1.00	5.38-04	2.03	1.72-02	3.12	1.07-01	4.26	3.48-01	20.77
75	612	1.00	5.08-04	2.03	1.63-02	3.12	1.02-01	4.25	3.32-01	20.26
76	627	1.00	4.81-04	2.03	1.55-02	3.11	9.71-02	4.24	3.18-01	19.77
77	642	1.00	4.55-04	2.03	1.47-02	3.11	9.24-02	4.24	3.04-01	19.31
78	658	1.00	4.30-04	2.02	1.38-02	3.11	8.75-02	4.23	2.89-01	18.84
79	674	1.00	4.06-04	2.02	1.31-02	3.10	8.29-02	4.23	2.75-01	18.39
80	690	1.00	3.85-04	2.02	1.24-02	3.10	7.93-02	4.22	2.64-01	17.97
81	707	1.00	3.64-04	2.02	1.19-02	3.10	7.58-02	4.21	2.53-01	17.54
82	725	1.00	3.43-04	2.02	1.12-02	3.09	7.19-02	4.21	2.41-01	17.10
83	742	1.00	3.25-04	2.02	1.07-02	3.09	6.86-02	4.20	2.30-01	16.71
84	760	1.00	3.07-04	2.02	1.01-02	3.09	6.52-02	4.20	2.20-01	16.31
85	779	1.00	2.90-04	2.02	9.60-03	3.08	6.20-02	4.19	2.09-01	15.92
86	798	1.00	2.74-04	2.02	9.10-03	3.08	5.89-02	4.19	2.00-01	15.54
87	818	1.00	2.59-04	2.02	8.62-03	3.08	5.60-02	4.18	1.90-01	15.16
88	838	1.00	2.45-04	2.02	8.17-03	3.07	5.32-02	4.18	1.81-01	14.79
89	858	1.00	2.32-04	2.02	7.76-03	3.07	5.07-02	4.17	1.73-01	14.45
90	879	1.00	2.19-04	2.02	7.37-03	3.07	4.82-02	4.17	1.65-01	14.10
91	901	1.00	2.07-04	2.01	6.99-03	3.07	4.58-02	4.16	1.58-01	13.76
92	923	1.00	1.96-04	2.01	6.64-03	3.06	4.35-02	4.16	1.50-01	13.43
93	945	1.00	1.85-04	2.01	6.32-03	3.06	4.14-02	4.15	1.44-01	13.12
94	968	1.00	1.75-04	2.01	6.00-03	3.06	3.94-02	4.15	1.37-01	12.81
95	992	1.00	1.66-04	2.01	5.70-03	3.06	3.74-02	4.14	1.30-01	12.50
96	1016	1.00	1.57-04	2.01	5.42-03	3.06	3.56-02	4.14	1.24-01	12.20
97	1041	1.00	1.48-04	2.01	5.13-03	3.05	3.38-02	4.13	1.18-01	11.91
98	1067	1.00	1.40-04	2.01	4.86-03	3.05	3.21-02	4.13	1.12-01	11.62
99	1093	1.00	1.32-04	2.01	4.61-03	3.05	3.05-02	4.12	1.07-01	11.34
100	1119	1.00	1.25-04	2.01	4.38-03	3.05	2.91-02	4.12	1.02-01	11.08
101	1147	1.00	1.18-04	2.01	4.15-03	3.05	2.76-02	4.12	9.69-02	10.81
102	1175	1.00	1.12-04	2.01	3.93-03	3.05	2.62-02	4.11	9.22-02	10.55
103	1204	1.00	1.06-04	2.01	3.73-03	3.04	2.49-02	4.11	8.77-02	10.30
104	1233	1.00	9.98-05	2.01	3.54-03	3.04	2.37-02	4.11	8.35-02	10.06
105	1263	1.00	9.43-05	2.01	3.36-03	3.04	2.25-02	4.10	7.95-02	9.82
106	1294	1.00	8.91-05	2.01	3.19-03	3.04	2.14-02	4.10	7.56-02	9.58
107	1326	1.00	8.41-05	2.01	3.03-03	3.04	2.03-02	4.10	7.19-02	9.35
108	1358	1.00	7.95-05	2.01	2.88-03	3.04	1.93-02	4.09	6.85-02	9.13
109	1392	1.00	7.50-05	2.01	2.73-03	3.03	1.83-02	4.09	6.51-02	8.91
110	1426	1.00	7.08-05	2.01	2.60-03	3.03	1.74-02	4.09	6.20-02	8.69
111	1460	1.00	6.70-05	2.01	2.47-03	3.03	1.65-02	4.08	5.91-02	8.49
112	1496	1.00	6.32-05	2.01	2.34-03	3.03	1.57-02	4.08	5.62-02	8.29
113	1533	1.00	5.97-05	2.01	2.21-03	3.03	1.48-02	4.08	5.34-02	8.09
114	1570	1.00	5.64-05	2.01	2.10-03	3.03	1.41-02	4.07	5.08-02	7.90
115	1609	1.00	5.32-05	2.01	1.98-03	3.03	1.34-02	4.07	4.83-02	7.71
116	1648	1.00	5.03-05	2.01	1.88-03	3.03	1.27-02	4.07	4.59-02	7.52
117	1688	1.00	4.76-05	2.01	1.78-03	3.03	1.20-02	4.07	4.37-02	7.34
118	1730	1.00	4.49-05	2.00	1.68-03	3.02	1.14-02	4.06	4.15-02	7.17
119	1772	1.00	4.24-05	2.00	1.59-03	3.02	1.08-02	4.06	3.95-02	7.00
120	1815	1.00	4.01-05	2.00	1.50-03	3.02	1.02-02	4.06	3.75-02	6.83
121	1860	1.00	3.78-05	2.00	1.41-03	3.02	9.70-03	4.06	3.56-02	6.67
122	1905	1.00	3.57-05	2.00	1.34-03	3.02	9.20-03	4.06	3.38-02	6.51
123	1952	1.00	3.37-05	2.00	1.26-03	3.02	8.71-03	4.05	3.21-02	6.35
124	2000	1.00	3.18-05	2.00	1.19-03	3.02	8.25-03	4.05	3.05-02	6.20

$\frac{E_p(E)}{f_2}$	41725	10507	6059.	4667.	$\frac{\text{keV-cm}^2}{\text{gram}}$
Atomic Weight	1.008	4.003	6.941	9.012	amu

Our complete work on the atomic scattering factors for the 100-2000 eV region is scheduled to appear in Atomic Data and Nuclear Data Tables 27, No. 1 (1982).

The interpolated tables for f_1 and f_2 , as illustrated here, will be in the Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics (November 1981).

The interpolated f_1 and f_2 data will also be available on a single-sided, single density 8" disk. Requests may be addressed to:

Professor Burton L. Henke
Low Energy X-Ray and Electron
Physics Project
University of Hawaii
Department of Physics and Astronomy
2505 Correa Road, Watanabe Hall
Honolulu, Hawaii 96822

N	E(eV)	Np (93) Neptunium		Pu (94) Plutonium		f_1	f_2	f_1	f_2	$\lambda(A)$
		f_1	f_2	f_1	f_2					
65	480	18.32	25.12	19.17	21.94					25.83
66	492	18.67	26.35	19.25	22.98					25.20
67	504	19.19	27.61	19.36	24.05					24.60
68	516	19.91	28.89	19.50	25.15					24.03
69	529	20.61	29.50	19.69	26.36					23.44
70	542	21.02	30.92	19.93	27.60					22.87
71	555	21.68	32.38	20.17	28.86					22.34
72	569	22.92	33.98	20.44	30.25					21.79
73	583	24.51	34.96	20.70	31.93					21.27
74	597	25.86	35.66	21.33	33.88					20.77
75	612	27.25	36.41	22.40	36.06					20.26
76	627	28.66	37.16	24.02	38.32					19.77
77	642	30.34	37.65	26.52	39.94					19.31
78	658	31.89	37.64	28.98	40.16					18.84
79	674	33.20	37.64	30.89	40.38					18.39
80	690	34.33	37.59	32.54	40.52					17.97
81	707	35.40	37.51	34.21	40.57					17.54
82	725	36.39	37.44	35.76	40.19					17.10
83	742	37.28	37.37	36.88	39.85					16.71
84	760	38.14	37.30	37.74	39.50					16.31
85	779	38.24	36.42	38.21	39.14					15.92
86	798	37.98	37.74	37.21	38.79					15.54
87	818	38.60	39.14	39.35	40.59					15.16
88	838	40.26	40.56	40.45	41.13					14.79
89	858	42.24	41.47	41.60	41.66					14.45
90	879	44.40	41.14	42.85	42.21					14.10
91	901	46.01	40.80	44.36	42.79					13.76
92	923	47.51	40.47	46.20	43.35					13.43
93	945	48.89	39.98	48.22	43.10					13.12
94	968	50.05	39.40	49.75	42.46					12.81
95	992	51.14	38.82	51.12	41.81					12.50
96	1016	52.07	38.23	52.27	41.17					12.20
97	1041	52.75	37.53	53.08	40.41					11.91
98	1067	53.39	37.37	53.85	40.25					11.62
99	1093	54.09	37.21	54.67	40.10					11.34
100	1119	54.87	37.06	55.58	39.95					11.08
101	1147	55.74	36.90	56.58	39.79					10.81
102	1175	56.63	36.75	57.60	39.64					10.55
103	1204	57.59	36.59	58.71	39.48					10.30
104	1233	58.68	36.44	59.96	39.33					10.06
105	1263	59.88	36.12	61.32	38.98					9.82
106	1294	61.00	35.40	62.60	38.17					9.58
107	1326	61.91	34.69	63.65	37.37					9.35
108	1358	62.72	34.02	64.58	36.60					9.13
109	1392	63.46	33.33	65.44	35.82					8.91
110	1426	64.09	32.67	66.20	35.08					8.69
111	1460	64.68	32.04	66.93	34.37					8.49
112	1496	65.22	31.42	67.64	33.63					8.29
113	1533	65.73	30.87	68.27	32.87					8.09
114	1570	66.23	30.34	68.86	32.13					7.90
115	1609	66.75	29.80	69.42	31.40					7.71
116	1648	67.23	29.29	69.92	30.69					7.52
117	1688	67.72	28.78	70.40	30.00					7.34
118	1730	68.23	28.28	70.87	29.31					7.17
119	1772	68.70	27.70	71.29	28.61					7.00
120	1815	69.15	27.11	71.69	27.91					6.83
121	1860	69.56	26.53	72.05	27.22					6.67
122	1905	69.88	25.97	72.33	26.56					6.51
123	1952	70.22	25.41	72.61	25.90					6.35
124	2000	70.57	24.86	72.89	25.26					6.20

$E_U(E)$
 I_2

177.4

172.4

$\frac{\text{keV-cm}^2}{\text{gram}}$

Atomic
Weight

237.0

244.0

amu

RESEARCH PUBLICATIONS (PUBLISHED OR IN PRESS)

1977 - 1981

57. "0.1 to 10 keV X-Ray-Induced Electron Emissions from Solids--Models and Secondary Electron Measurements," *J. Appl. Phys.* 48, 1852 (1977) (w/ J. A. Smith and D. T. Attwood).
58. "High Efficiency Low-Energy X-Ray Spectroscopy in the 100-500 eV Region," *J. Appl. Phys.* 49, 480 (1978) (w/ R. C. C. Perera, E. M. Gullikson and M. L. Schattenburg).
59. "Cl-L_{II,III} Fluorescent X-Ray Spectra Measurement and Analysis for the Molecular Orbital Structure of ClO₄, ClO₃ and ClO₂," *J. Chem. Phys.* 68, 3692 (1978) (w/ R. C. C. Perera and D. S. Urch).
60. "Some Recent Studies in Low Energy X-Ray Physics," *Proceedings of the 8th International Conference on X-Ray Optics and Microanalysis* (Boston, August 1977).
61. "Models and Measurement for the Response of Dielectric X-Ray Photocathodes," Scientific Reports, AFOSR 75-2762-F and DOE E(04-3)235-PA15, March 1978.
62. "Low Energy X-Ray Emission Spectroscopy in the 100-500 eV Region: Molecular Orbital Interpretation," (PhD Thesis by R. C. C. Perera) Special Scientific Report, AFOSR 75-2762-F, May 1978.
63. "The Secondary Electron Emission Photocathode Characteristics for Time Resolved X-Ray Spectroscopy," *Proceedings of the International Conference on X-Ray and XUV Spectroscopy* (Sendai, Japan, August 1978); *Jap. J. Appl. Phys.* 17, Suppl. 17-2, p. 23 (1978) (w/ K. Premaratne).
64. "C-K and Cl-L Emission Spectra and Molecular Orbital Analysis of CCl₄" *Proceedings of the International Conference on X-Ray and XUV Spectroscopy* (Sendai, Japan, August 1978); *Jap. J. Appl. Phys.* 17, Suppl. 17-2, p. 23 (1978) (w/ R. C. C. Perera).
65. "A Soft X-Ray Spectrometer for the Study of Plutonium and Plutonium-based Materials," *X-Ray Spectrometry* ? (1978) (w/ P. L. Wallace, W. L. Haugen and E. M. Gullikson).
66. "Soft X-Ray Induced Secondary Electron Emission from Semiconductors and Insulators: Models and Measurements," *Phys. Rev.* B19, 3004 (1979) (w/ J. Liesegang and S. D. Smith).
67. "Low Energy X-Ray Emission Spectra and Molecular Orbital Analysis of CH₄, CCl₄ and CHCl₃," *J. Chem. Phys.* 70, 5398 (1979) (w/ R. C. C. Perera).
68. "The Characterization of Photocathodes for Application to Time-Resolved X-Ray Spectroscopy," Technical Progress Report, AFOSR 79-0027 and DOE DE-AS03-76SF00235, April 1979.

69. "Multilayer X-Ray Spectrometry in the 20-80 Å Region: A Molecular Orbital Analysis of CO and CO₂ in the Gas and Solid States," *X-Ray Spectrometry* 9, 81 (1980) (w/ R. C. C. Perera).
70. "X-Ray Spectrometry in the 100-1000 eV Region," *Nucl. Instrum. Methods* 177, 161 (1980).
71. "Evaluation of High Efficiency CsI and CuI Photocathodes for Soft X-Ray Diagnostics," *Appl. Opt.* 19, 748 (w/ E. B. Saloman and J. A. Pearlman).
72. "The Characterization of X-Ray Photocathodes in the 0.1-10 keV Photon Energy Region," *J. Appl. Phys.* 52, 1509 (1981) (w/ J. P. Knauer and K. Premaratne).
73. "Low Energy X-Ray Interaction Coefficients: Photoionization, Scattering and Reflection," *Atomic Data and Nuclear Data Tables* 27, No. 1 (1982) (w/ P. Lee, T. J. Tanaka, R. L. Shimabukuro and B. K. Fujikawa).
74. "X-Ray Diffraction in Multilayers," *Opt. Commun.* 37, 159 (1981) (Ping Lee).
75. "Low Energy X-Ray Spectroscopy with Crystals and Multilayers," *Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics* (November 1981).
76. "A Sensitometric Calibration of the RAR 2497 Film for the Low Energy X-Ray Region," *Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics* (November 1981) (w/ E. R. Dietz, T. S. Durland, and M. A. Tester).
77. "Low Energy X-Ray Interactions: Photoionization, Scattering, Specular and Bragg Reflection," *Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics* (November 1981).
78. "Appendix: The Atomic Scattering Factor, $f_1 + if_2$, for 94 Elements and for the 100 to 2000 eV Photon Energy Region," *Proceedings of the 1981 Topical Conference on Low Energy X-Ray Diagnostics* (November 1981) (w/ P. Lee, T. J. Tanaka, R. L. Shimabukuro and B. K. Fujikawa).
79. "The Stability of Cesium Iodide X-Ray Photocathodes," *Appl. Phys. Letters*, to be published (w/ K. Premaratne and E. R. Dietz).

INVITED AND CONTRIBUTED RESEARCH PAPERS
PRESENTED BY THE PRINCIPAL INVESTIGATOR

1977 to 1981

1977

- Seminar at Lawrence Livermore Laboratory, Livermore, California, August 1977
- Seminar at Los Alamos Scientific Laboratory, Los Alamos, New Mexico, August 1977
- Eight International Conference on X-Ray Optics and Microanalysis, Boston, Massachusetts, August 1977

1978

- *A Systematic Study of the Characteristics of X-Ray Photocathodes*, Poster presentation, American Physical Society Second Topical Conference on High Temperature Plasma Diagnostics, Santa Fe, New Mexico, February 28 - March 3, 1978
- *Application of Low Energy X-Ray Spectroscopic Techniques to High Temperature Plasma Diagnostics*, Physics seminar lecture, Los Alamos Scientific Laboratory, June 1978
- *The Optimization of X-Ray Photocathodes for Time Resolved X-Ray Spectroscopy in Laser-Produced Fusion Research*, Physics colloquium lecture, University of California Lawrence Livermore Laboratory, June 1978
- Participated in a workshop on the Absolute Calibration of X-Ray Photocathodes as Applied in X-Ray Detectors (XRD's) sponsored by the National Bureau of Standards at the Lawrence Livermore Laboratory, June 1978. The results of the calibrations of two detectors that were calibrated by each of the six participating laboratories, including this one, were evaluated.
- *The Secondary Electron Emission Photocathode Characteristics for Time Resolved X-Ray Spectroscopy*, International Conference on X-Ray and XUV Spectroscopy, Sendai, Japan, August 28 - September 1, 1978
- *U-2 and Cl-L Emission Spectra and Molecular Orbital Analysis of CCl₄*, International Conference on X-Ray and XUV Spectroscopy, Sendai, Japan, August 28 - September 1, 1978
- *A Review of X-Ray Photocathode Characteristics that Affect Picosecond Streak Camera Operation*, 1978 American Physical Society Annual Meeting of the Division of Plasma Physics, Colorado Springs, October 30 - November 3, 1978
- *Physics and Application of Multilayer 'Crystals' for Spectral Analysis in the 50-100 Å Region*, Invited paper, American Crystallographic Assn. Meeting (Joint with Japanese Crystallographic Society), Honolulu, Hawaii, March 26-30, 1979.

1979

- Seminar at Lawrence Livermore Laboratory, June 20, 1979
- Seminar at Los Alamos Scientific Laboratory, June 26, 1979
- Seminar at Kirtland Air Force Base and Sandia Laboratories, Albuquerque, New Mexico, June 28, 1979
- Seminar at Maxwell Laboratories, Inc., San Diego, June 29, 1979
- *X-Ray Spectroscopy in the 100-1000 eV Region*, Invited review paper, Japan-U.S.A. Seminar on Synchrotron Radiation Facilities, East-West Center, University of Hawaii, November 5-9, 1979
- *The Characterization of X-Ray Photocathodes*, 21st Annual Meeting of the Division of Plasma Physics, American Physical Society, Boston, November 12-16, 1979
- Seminar at Department of Physics, Pomona College, Claremont, California, November 1979
- Seminar at Massachusetts Institute of Technology, Center for Space Research, Cambridge, Massachusetts, November 1979

1980

- Seminar at Lawrence Livermore Laboratory, August 1980
- Seminar at Los Alamos Scientific Laboratory, August 1980
- Seminar at Kirtland Air Force Base and Sandia Laboratories, Albuquerque, New Mexico, August 1980
- *Some Recent Developments in Low Energy X-Ray Spectroscopy*, 1980 Annual Meeting of the Division of Plasma Physics, American Physical Society, San Diego, November 10-14, 1980

1981

- Co-organizer of a special Topical Conference on Low Energy X-Ray Diagnostics sponsored by the American Physical Society, June 8-10, 1981, Monterey, California. Contributions for this program include the following:

1. *Low Energy X-Ray Spectroscopy with Crystals and Multilayers.*
2. *Low Energy X-Ray Interactions: Photoionization, Scattering, Specular and Bragg Reflection.* (Review paper)
3. *An Absolute Calibration of RAR 2497 Film for Low Energy X-Ray Spectroscopy.* (with E. R. Dietz and M. A. Tester) (Review paper)
4. *The Atomic Scattering Factor, $f_1 + if_2$, for 94 Elements and for the 100 to 2000 eV Photon Energy Region.* (with P. Lee, T. J. Tanaka, R. L. Shimabukuro and B. K. Fujikawa).

Proceedings of this Conference will be published by the American Institute of Physics.

**TOPICAL CONFERENCE ON
LOW ENERGY X-RAY
DIAGNOSTICS
Monterey, California
8-10 June 1981**

The meeting will provide a forum for active researchers in differing scientific fields to meet and discuss common interests in the rapidly evolving technologies of low energy (100 eV to 1 KeV) x-ray generation, manipulation, and detection, as well as the physical phenomena these developments make accessible. Papers are solicited in the areas of low energy x-ray sources, detectors and spectroscopy, as well as reflective and diffractive optics. The meeting is expected to emphasize, through invited papers, new developments in microfabrication techniques, applications to the diagnosis of high density, high temperature plasmas, and x-ray lithographic applications in science and industry. Conference Co-chairmen are David Attwood of the Lawrence Livermore National Laboratory and Burton Henke of the University of Hawaii. The meeting is jointly sponsored by the American Physical Society, the U. S. Department of Energy, and the Lawrence Livermore National Laboratory.

Because only a small number of rooms have been reserved in this popular tourist region, participants are urged to reserve rooms quickly and directly at the Doubletree Inn, Monterey, California [telephone: (408) 649-4511]. In doing so, refer to the "X-Ray Conference". Further information regarding presentation of papers, program details, and preregistration can be obtained by writing to David T. Attwood, P. O. Box 5508, L-479, Lawrence Livermore National Laboratory, Livermore, Calif. 94550. The registration fee of approximately \$60 includes a subsequent copy of the meeting's proceedings, bound in book form by the American Institute of Physics. All presentations must be available in camera-ready form at the time of the meeting, to APS journal standards, for inclusion in the published proceedings. ■

**FIRST-PAGE ABSTRACTS OF
RESEARCH PUBLICATIONS
1977 - 1981**

0.1-10-keV x-ray-induced electron emissions from solids—Models and secondary electron measurements

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Analytical models are presented describing the x-ray-excited emission of "no-loss" photoelectrons and Auger electrons and the energy distribution of emitted secondary electrons. The secondary electron energy distribution is given in terms of the electron kinetic energy E_k , work function ϕ , photon energy E_γ , and mass photoionization coefficient $\mu(E_\gamma)$, as proportional to $E_k \mu(E_\gamma) E_k (E_k + \phi)^{-4}$. Techniques of electron spectral measurements utilizing uniform field preacceleration and limited acceptance angle spectrometers are discussed. Secondary electron energy distributions are measured at about 10^{-8} Torr from thick evaporated films of gold and aluminum at photon energies 277, 1487, and 8050 eV. The shapes of these distributions do not depend significantly upon photon energy. The full width at half-maximum (FWHM) of these distributions are 3.9, 6.7, and 4.4 eV for Au and ion-cleaned Au and Al photocathodes, respectively. The data agree well with the model predictions.

PL CS numbers: 79.60.Cn, 71.30.+y, 72.10.Bz

I. INTRODUCTION

This work is in sequel to and in support of a recent presentation by the authors of some measurements on the secondary electron energy distributions from gold as excited by C-K α (277 eV) and Al-K α (1487 eV) x-ray photons.¹ It is an attempt to present the basic physics for the measurement and for the interpretation of the x-ray-induced electron emissions from uniform isotropic solid.

In Fig. 1 are shown the typical characteristics of an electron spectrum induced by an x-ray beam incident upon a solid. Illustrated here are the sharp photoelectron and Auger electron "no-loss" lines with their characteristic energy loss tail structure, along with the low-energy secondary electron distribution. In contrast to uv-excited electron spectra, here the photoelectrons and the principal sharp Auger electron emissions are well outside the low-energy secondary electron energy region. The secondary electron spectrum peaks at about 1 to 2 eV and has a full width at half-maximum (FWHM) that is usually below 10 eV. In this 0–30 eV interval are typically from 50 to 90% of the total number of electrons emitted for photon excitation in the 100–10000-eV region.

The x-ray-excited electron spectra constitute a unique "window" into the solid and its electron excitation, transport, and escape processes. When a thorough understanding of the physics of these processes is gained, electron spectroscopy can provide an important quantitative basis for the physical and chemical analysis of solids. The electron spectroscopy for chemical analysis (referred to as ESCA or XPS) has become a well-researched area within the last ten years.²

The photoelectric conversion of x-ray intensity into electron emission can provide an important practical basis for x-ray intensity measurement. X-ray photoelectric detectors are vacuum devices and, unlike gas ionization detectors, can be windowless. A unique advantage of the photoelectric detector is that it can be

applied effectively over a wide band of photon energies.^{3,4}

A very recent application of secondary electron detectors has been in the development of streak and framing cameras for the diagnostics of x-ray bursts from laser-produced plasmas. The time spread in the photoconverted secondary electron emission per photon is probably of the order of 10^{-14} sec, and the energy spread is of the order of 10 eV. An x-ray source can be imaged and photoconverted to an electron source which may then be reimaged down a streak or framing camera tube with an accelerating electron lens system. The time history of an x-ray event can be obtained by a fast transverse deflection of this image, e.g., to form a "streak" pattern with a time resolution in the picosecond range.^{1,5-7}

In order to support research and application in x-ray photoemission, considerably more theoretical and experimental work should be done on the development of a quantitative relationship between the electron emission spectrum, the incident photon energy, and the characteristics of the photocathode. There is no complete theory of x-ray photoemission that is available

FIG. 1. A typical x-ray-excited photoemission spectrum.

Proceedings of the Eighth International Conference on X-Ray Optics and Microanalysis, Boston, August 1977.

SOME RECENT WORK IN LOW ENERGY X-RAY PHYSICS. B. L. Henke
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1. X-Ray Sources--High intensity, monochromatic excitation sources are essential for quantitative studies of the emission processes for photoelectrons, Auger and secondary electrons and for fluorescent x-rays. Such sources are also needed for the calibration of the detectors and analyzers employed for these studies and for subsequent applications. In the low-energy x-ray region (10-100 Å/100-1000 eV) the direct radiation from an x-ray tube anode, with the appropriate filter and anode voltage, may be sufficiently monochromatic because the line radiation often dominates the associated continuum radiation. The line-continuum profiles have been measured and will be presented here for several useful K, L, and M characteristic line sources in order to illustrate the effect of filters and anode voltage. The absolute brightness of these sources (in photon/sec-stereadian) will also be presented.

2. Electron Spectroscopy--The electron spectroscopy of x-ray produced photoemissions has recently become an important tool in surface analysis. Photoelectron and Auger electron spectroscopy most effectively probe core electron states and the secondary electron spectroscopy probes the valence electron band states of the surface material. The basic processes that determine the photoemission spectra are the excitation, transport and the escape processes. In order that electron spectroscopy can be fully realized as a quantitative tool, considerably more must be known of the physics of these processes. This is particularly the case for secondary electron emission which is the most complex and for which there is no complete theory at this time.

Theoretical model results will be presented here along with examples of recently measured secondary electron energy distributions of metals and dielectrics. The secondary emission spectra rise sharply from zero electron kinetic energy to a peak value of about one eV and with a FWHM usually in the two to five eV region. These are being measured with a resolution of .04 eV using a hemispherical electrostatic analyzer. A uniform pre-acceleration field is employed which permits the application of a simple and accurate correction for a change in electron optical brightness associated with preacceleration (acceptance energy of the spectrograph is set at 15 volts).

It is hoped that measurements as these will also be helpful in gaining a more complete understanding of the secondary electron contrast dependence upon the surface state in scanning electron microscopy, and in the choice of x-ray photocathode materials particularly as used for pulsed x-ray measurements for temporal resolutions in the picosecond region.

3. X-Ray Spectroscopy--The low energy x-ray spectroscopy has been demonstrated to be a very useful tool for light element analysis, valence band and molecular orbital analysis, and for high temperature plasma diagnostics. The light elements emit only in the long wavelength x-ray region. Spectra from all elements involving transitions from the valence or molecular orbital levels to the nearby, relatively sharp core levels are in the one-to-several hundred eV region and do sensitively portray important outer electronic state structure. Plasma in the ten-million degree range (astrophysical and CTR, for example) emit most strongly in the low energy x-ray region. To accomplish this type of x-ray spectroscopy, the simpler and higher efficiency crystal spectroscopy is sometimes more appropriate than the grating spectroscopy even though the latter is inherently capable of higher resolution.

Presented here will be some examples of atomic and molecular, fluorescent spectroscopy of gaseous and solid samples using the multilayer analyzer (Langmuir-Blodgett type). The measured reflection coefficients and resolution for the lead myristate crystal will be presented in detail. And a simple method for unfolding the spectrographic lines and for decomposing overlapping spectra in order to gain spectral resolutions in the 0.5 eV range will be described.

High-efficiency low-energy x-ray spectroscopy in the 100-500-eV region

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The lead myristate multilayer analyzer has provided a basis for a relatively simple and efficient spectroscopy for the low-energy x-ray emissions in the 20-80-Å region (where conventional crystal spectroscopy and grazing incidence grating spectroscopy are generally inefficient). The percent reflectivity, the integrated coefficient of reflection, and the Bragg diffraction width of the lead myristate analyzer have been measured and found to be consistent with the predictions of a simple theoretical model for multilayer diffraction. This multilayer spectroscopy at large Bragg angles has a high efficiency (high instrument transmission) as compared to grazing incidence grating spectroscopy in this 20-80-Å region. However, the resolution is limited to that set by the diffraction width of the lead myristate analyzer of about 1 eV. Because the collimator-crystal broadening function can be precisely defined, a simple and effective deconvolution procedure can be applied with this multilayer spectroscopy to bring the resolution into the sub-electron-volt region. To demonstrate the efficiency of lead myristate spectroscopy in the 20-80-Å region, spectra were measured and analyzed from x-ray excited fluorescent sources which are characteristically of low intensity. (X-ray excitation yields a minimum of background spectra and of radiation damage.) These include the $L_{2,3}$ atomic spectrum of argon and the C-K molecular spectrum of CO_2 , both in the gas phase, and the Cl- $L_{2,3}$ and O-K spectra from solid lithium perchlorate. Many samples undergo appreciable radiation-induced chemical change during the exposure time that is required for measurement—even with an optimally fast spectrograph and with fluorescent excitation. A method has been developed to evaluate and to correct for radiation damage by distributing the exposure over an effectively large sample volume either by gas flow or by rotating through multiple samples during measurement. Several spectral scans were made on the LiClO_4 using six samples. The total exposure time for each data point in each scan was recorded which permitted an extrapolation into a "zero" exposure spectrum. Finally, Fe- $L_{2,3}/\text{O-K}$ spectrum (from Fe_2O_3) in the 17-25-Å region is presented to illustrate the effectiveness of the lead myristate analyzer in third-order diffraction. For this multilayer, the third-order diffraction efficiency is one-third that of the first order and is nearly twice that of the second order for this wavelength region.

PACS numbers: 07.85.+n, 32.30.Rj, 32.70.Kz, 33.20.Rm

I. INTRODUCTION

There are two areas in which low-energy x-ray spectroscopy is of particular importance at this time—the diagnostics of high-temperature plasmas¹ and the determination of the chemical and solid-state electronic structure of atomic systems.²

In the controlled thermonuclear fusion research, a critical temperature region of current interest is in the $(1-10) \times 10^6$ °C range. The plasmas involved emit radiations most characteristically in the low-energy x-ray region (100-1000 eV/10-100 Å). The detailed spectroscopy of these plasma radiations can yield information as to the plasma density, temperature, and the identity and amount of contaminating elements. The low-energy x-ray radiation from pulsed plasma sources (as produced by lasers or exploding wires) can be very efficiently converted to relatively sharp distributions in energy of secondary electrons³ that are amenable, with streak camera techniques, to time-history measurements approaching picosecond resolutions.

Often, the energy and the symmetry of the outer electronic states of atomic systems can be sensitively revealed through the spectra associated with the transitions from these states into a nearby relatively sharp core level. Such spectra can yield valuable data complementary to that which are available from photoelectron Auger electron spectroscopy on the structure of valence bands, solid-state bands, and molecular orbitals.⁴ These sensitive first transitions into

the core levels typically result in low-energy x-ray spectra at a few hundred eV or less.

Using, for example, the acid phthalate crystals (2d value of about 26.6 Å), the conventional x-ray crystal spectroscopy has been very effectively extended down to about 300 eV.⁵ Extreme ultraviolet diffraction grating spectroscopy has been extended with high efficiency (with relatively large angles of grazing incidence) up to about 100 eV.⁶ We have found that a very efficient spectroscopy in the gap region of 100-500 eV is by using the multilayer analyzers as the lead stearate and lead myristate of 2d values equal to 160 and 80 Å, respectively. We have recently presented the detailed characteristics and application of the lead stearate analyzer.^{7,8} In this paper, we extend the presentation of the methods and techniques of low-energy x-ray spectroscopy as specially applied with the lead myristate analyzer.

In Secs. II-V, we present an analysis and measurements of the x-ray optical characteristics of this multilayer analyzer, an optimized spectroscopic and data analysis procedure for gaining maximum overall efficiency and resolution, and, finally, we present some examples of applications to atomic and molecular low-energy x-ray spectroscopy.

II. REFLECTION PARAMETERS FOR THE LEAD MYRISTATE MULTILAYER

Lead salts of the fatty acids deposited as Langmuir-Blodgett multilayers have been demonstrated to be highly efficient

Cl- $L_{II,III}$ fluorescent x-ray spectra measurement and analysis for the molecular orbital structure of ClO_4^- , ClO_3^- , and ClO_2^-

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The chlorine $L_{II,III}$ low energy x-ray spectra from sodium perchlorate, chlorate and chlorite have been obtained using carbon K_α (277 eV) photon excitation and a lead myristate analyzing "crystal" ($2d = 80$ Å). X-ray induced decomposition was observed for each of these compounds. By taking repeated spectral scans, systematically distributed over six samples, it was possible to extrapolate to "zero-dose" Cl- $L_{II,III}$ spectra. A specially developed least-squares fitting program was applied to precisely determine the energy and strength of each spectral component which utilized the known collimation and crystal broadening functions and yielded energy resolutions of less than 1 eV. Broad low-energy satellite structures were observed for all the oxy-anions and for chloride (NaCl) and have been compared to similar satellites as measured in the Ar- $L_{II,III}$ spectrum. These structures were thus identified as resulting from multielectron processes. The other peaks in the Cl- $L_{II,III}$ spectra of the oxy-anions could be understood as corresponding to transitions from molecular orbitals with Cl 3s or 3d character. These results have demonstrated that 3d orbitals do play a definite role in the formation of chemical bonds in the oxy-anions of chlorine and that the importance of this role increases with the oxidation state of the chlorine. Satisfactory correlations have been obtained with the complementary K_α x-ray emission and photoelectron spectra and with molecular orbital theory for the same anions.

I. INTRODUCTION

Transitions between the molecular orbital states and the nearby and relatively sharp core level states result in low energy x-ray spectra that typically lie in the 100-300 eV (40-100 Å) region. Such spectra can sensitively portray the orbital structure of the molecule (or, in many cases, of an ionic group). For the second-row elements, the nearest core levels are the $2p_{1/2}-2p_{3/2}$ spin-orbit split states. The atomic binding energies of these $L_{II,III}$ levels, for example, for 15 P, 16 S, 17 Cl, and 18 Ar are 136-135, 165-164, 202-200, and 247-245 electron volts, respectively. In a particular chemical environment, these core levels of a given atom may shift as much as 10 eV. Such core level chemical shifts can be measured by x-ray photoelectron spectroscopy (XPS). The molecular orbital energies are of the order of 10 eV and can also be measured directly by ultraviolet photoelectron spectroscopy (UPS). The x-ray emission spectra directly yield the difference in the energy of the molecular orbitals and the core level states. However, unlike the photoelectron spectra, the x-ray emission spectra reveal appreciable information about the symmetries of the molecular orbital states. The $L_{II,III}$ spectral intensities are determined mostly by the s and d character of the orbitals and the K_α spectral intensities are determined mostly by the p character of the orbitals. If the $L_{II,III}$ or K_α spectrum originates from an atom of a molecule or of a strongly ionic group that contains only one such atom, it is then relatively easy to approximately calculate the energy and the relative intensity of the x-ray spectral components. Such theoretical predictions can simply be based upon one-electron integrals with the molecular orbital states described as linear combinations of the s, p, and d

atomic orbital functions (LCAO approximation). The calculated eigenvectors are used to obtain the dipole transition probabilities. From such MO calculations the relative amounts of s, p, and d contribution can readily be estimated.

In an earlier work, Henke and Smith¹ were able to demonstrate the feasibility of obtaining the $L_{II,III}$ spectra of phosphorous, sulfur, and chlorine in different chemical states by applying spectrographic techniques of such efficiency as to minimize the effects of radiation decomposition. Recently, the S- $L_{II,III}$ spectra have been more precisely measured and analyzed by Henke and Taniguchi^{2,3} for the SO_3^{2-} and SO_4^{2-} ions for polycrystalline samples and for the molecules containing single sulfur atoms and in the gas or vapor states— H_2S , SO_2 , SF_6 , $\text{C}_4\text{H}_8\text{S}$. The molecular orbital information derived from these spectra were compared to that obtained from the complementary photoelectron and K_α spectroscopy and to the predictions of molecular orbital theory. In this present work, the Cl- $L_{II,III}$ spectra for the ClO_2^- , ClO_3^- , and ClO_4^- ions for polycrystalline samples are measured, analyzed and compared to the photoelectron, K_α , and MO calculated⁴ data for the same ionic systems. Also, important comparisons with the measured atomic $L_{II,III}$ spectra for Ar and NaCl are presented.

A striking difference in the experimental determinations of the $L_{II,III}$ spectra of the sulfur and the chlorine compounds has been that the latter undergo considerably greater chemical change as induced by the excitation radiation that is required for the spectral measurement. That radiation decomposition might be important in the soft x-ray spectra of chloro-anions had been discussed by Best⁵ in the electron excitation of Cl K_α spectra and had also been suggested by Urch⁶ in attempting to interpret the early spectra of Henke and Smith.¹ Subsequently, both Prins⁷ in x-ray photoelectron experiments and Sadoyskii *et al.*⁸ in measuring Cl- $L_{II,III}$ emission

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The Secondary Electron Emission Photocathode Characteristics for Time Resolved X-Ray Spectroscopy

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Recently the secondary electron energy distributions and the relative secondary electron yields for the 0.1 to 10 keV photon excitation region have been measured for gold, aluminum and for sixteen representative semiconductors and insulators (alkali halides), and a simple phenomenological model for X-ray photoemission has been developed. This work is discussed here as it might be applied to the application of streak cameras for time resolved X-ray spectroscopy.

§1. Introduction

Time resolved X-ray spectroscopy has recently become of considerable value in studies of high temperature plasmas in the one second range (magnetically confined fusion) to the picosecond range (laser produced fusion). Mode-locked laser systems are available that can generate high intensity pulses of X-radiation from matter in the picosecond region. Ultra-fast spectroscopy is needed for the characterization of such X-ray sources and of the effects of their radiation bursts upon materials. Pico second X-ray spectroscopy may be a valuable tool for the measurement of the lifetimes of metastable atomic and molecular states and of certain photochemical processes.¹⁻³⁾

A proven method for accomplishing time resolved X-ray spectroscopy is that with the X-ray streak tube.⁴⁻⁶⁾ An X-ray beam is dispersed according to its photon energy along a slit-defined photocathode using a non-focusing crystal or a diffraction grating (or by a series of absorption filter and/or total-reflection monochromator channels). The secondary electrons from this slit source are used to form a line image at an image intensifier (needed particularly for ultra-fast spectroscopy). This line image is "streaked" to establish a time base using a pair of deflecting plates. The optical output of the image intensifier is recorded photographically. A schematic of such an X-ray streak tube is shown in Fig. 1. As indicated here, two types of imaging can be used, either an electron lens system^{7,8)} or a simple, proximity-focusing microchannel plate

Fig. 1. Schematic of an X-ray streak tube as applied for time resolved X-ray spectroscopy. The temporal resolution limit, T , is the difference in arrival time at the image intensifier for axially emitted electrons from the photocathode of initial velocities equal to zero and to v_0 . The corresponding energy spread, Δ , of the secondary electron emission is $1/2 \cdot mv_0^2$.

system.^{9,10)}

The intensity-and-photon-energy response and the temporal resolution of the streak camera are ultimately determined by the characteristics of the photocathode. In the sections that follow, we have attempted to review (1) the basic relationship between the photoemission and the electron-optical characteristics of the X-ray streak tube, and (2) the experimental and theoretical determination of the relevant photoemission properties of metal and dielectric X-ray photocathodes as have been recently investigated in this laboratory.¹¹⁻¹³⁾

Soft-x-ray-induced secondary-electron emission from semiconductors and insulators: Models and measurements

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Secondary-electron energy distribution curves (EDC's) and the total secondary-electron yields relative to such for gold have been measured for seven semiconductors for which electron-electron scattering losses within the emitter were considered dominant and for nine insulators (alkali halides) for which electron-phonon scattering losses were expected to be dominant in the transport process. The secondary-electron spectra were excited by Al-K α (1487 eV) photons and were measured from evaporated dielectric films (of about 0.3 μ thickness) on conducting substrates with an electrostatic hemispherical analyzer of about 0.03-eV resolution. Some of the dielectric photoemitters have appreciably narrower energy distributions and higher yields than has gold; CuI and CsI have EDC widths at half-maximum of about one-third of that for gold, and yield values of 11 and 30 times greater. The FWHM and secondary-electron yield for gold were measured to be about 4 eV and 0.50 electrons per normally incident photon, respectively. The shapes of the EDC's were found to be essentially unchanged for photon excitation in the 0.1-10-keV region. Strong structural features appear only in the alkali halide EDC's, and it is proposed that these are mainly the result of single-electron promotion of secondaries from the valence band by plasmon deexcitation. A relatively simple model for x-ray photoemission has been developed which assumes that direct excitation of secondaries by photoelectron and Auger-electron "primaries" is the dominant excitation mechanism, and accounts for both electron-electron and electron-phonon scattering in the transport process. Free-electron conduction-band descriptions are assumed. The theoretical and experimental curves are in satisfactory agreement.

1. INTRODUCTION

There has been a considerable amount of effort on the theory and application of secondary-electron emissions using electron excitation in the kilovolt region (as applied, for example, in scanning microscopy) and using extreme ultraviolet excitation (as applied in band-structure analysis). There has been relatively little theoretical or experimental work reported on the generation of the secondary electrons using x-ray excitation (which is of considerable current interest as applied to the measurement of the intensity and the temporal history into the picosecond region of pulsed x-ray sources with the diode detector, the streak, and the framing cameras in high-temperature plasma diagnostics).

With electron and extreme ultraviolet generation of the secondary-electron distribution, the effective escape depths of the electrons can be very dependent upon the attenuation mechanism of the exciting radiation. With x-ray excitation of the photoelectron and subsequent emission of the associated Auger-electron "primaries" which in turn generate the internal secondary-electron distribution, the electron escape depths are usually independent of the x-ray attenuation process. This is because the x-ray penetration is very large as compared to the effective electron escape length. Thus with x-ray excitation, often a more direct and precise interpretation of the secondary-electron energy

distribution can be made in terms of models for the excitation, transport, and escape processes.

In an earlier work,¹ the electron energy dependence of the secondary-electron energy distribution from metals as excited by x-rays in the 0.1-10-keV region was measured and found to be consistent and predictable by applying currently available theoretical descriptions for the excitation, mean free paths, and escape for secondaries in metals. In this present work, we have measured the energy dependence and relative yields of the secondary electrons as excited by soft x rays (principally at 1487-eV photon energy) for a representative series of semiconductors and insulators. For these systems, the secondary-electron generation processes are more complex, particularly for the insulators for which multiple scattering has an appreciable role in the transport process. In order to test available theoretical expressions for the secondary-electron excitation and for the mean free paths for pair production and for electron-phonon interactions for the energy region below 10 eV, we have used the relatively simple rate equation developed by Kane² for a description of the multiple scattering transport process. We believe this approach will be helpful at this time in guiding the application of more exact transport theories, analytical and numerical, in later studies.

In Sec. II, we present the "semiclassical," simple case for x-ray excited secondary-electron generation for the "no-loss" transport (no multi-

C-K and Cl-L Emission Spectra and Molecular Orbital Analysis of CCl_4

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The C-K and $\text{Cl-L}_{II,III}$ low energy X-ray spectra from solid CCl_4 have been obtained using monoenergetic X-ray excitation and a lead myristate multilayer analyzing crystal. The Cl-L spectra was also measured in the vapor phase and compared with that measured in the solid phase. The deconvoluted C-K and $\text{Cl-L}_{II,III}$ spectra are compared with the available $\text{Cl-K}\beta$ and UPS spectra and with the results of CNDO/2, MINDO/3 and extended Hückel MO calculations.

§1. Introduction

The X-ray emission spectra from gaseous chlorinated methane derivatives have been previously reported by many authors. LaVilla and Deslattes¹⁾ studied the chlorine-K β emission spectra and Ehlert and Mattson²⁾ reported the carbon-K and chlorine-L spectra from four chlorinated derivatives of methane. The photoelectron spectra of chloromethanes were measured by Potts *et al.*³⁾ using 21 eV and 40 eV excitations and by Turner *et al.*⁴⁾ using 21 eV excitation. The experimental photoelectron spectra are in good agreement. Hopfgarten and Manne⁵⁾ provided a molecular orbital interpretation of available photoelectron and X-ray emission spectra of chloromethanes on the basis of the extended Hückel molecular orbital calculations.

In this laboratory,^{6,7)} the C-K and Cl-L emission spectra of CCl_4 and CHCl_3 and the C-K emission spectra of CH_4 were measured in the solid phase. The C-K emission spectra of methane and the Cl-L emission spectra of chloromethanes were also measured in the gas phase. Molecular orbital analysis of these chloromethanes were based upon the CNDO/2 and MINDO/3 SCF-MO calculations and upon results of available extended Hückel MO calculations.⁵⁾ As an example, the spectra and molecular orbital analysis of CCl_4 will be presented here.

§2. Experimental

Basic details of the experimental approach have been given elsewhere.^{7,8)} For high efficiency, an oxidized copper excitation source was used to create the C-1s hole and a carbon excitation source was used to create the Cl-2p hole. The X-ray tube was operated at 8 kV and 150 mA. A lead myristate multilayer⁹⁾ was used as the analyzer. A "pressure tuned"⁹⁾ constant flow proportional counter filled with propane at subatmospheric pressure was used as the detector.

In measuring the chlorine-L_{II,III} spectra in the vapor phase, the sample pressure in the gas cell was maintained at one Torr for maximum intensity.¹⁰⁾ The chlorine-L_{II,III} spectra of CCl_4 in the solid and vapor phases were measured under the same excitation and are presented in Fig. 1. As seen from Fig. 1, there are no substantial differences between the gas phase and solid phase spectra. Since the fluorescent intensity from the solid phase was about ten times higher than in the gas phase, the spectra from the solid samples were used in the detailed analysis presented here.

Reagent grade CCl_4 was obtained commercially with better than 99% purity. All of the spectra presented in this work are the sum of at least three repeated runs and the individual runs reproduced within statistical deviations. Over 10^4 counts were collected at the peak in all spectra and the spectrometer was calibrated using Rh, Mo and Nb M γ lines.^{7,8)} In all of the spectra, the peak intensities were normalized and background was not subtracted from the data because it was negligibly small.

A step-scanned spectrum thus obtained was

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Evaluation of high efficiency CsI and CuI photocathodes for soft x-ray diagnostics

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The photoefficiency of CsI and CuI photocathodes was measured for photons in the 22-240-eV (50-560-Å) energy range. The within-batch and batch-to-batch variation in photoefficiency were studied as was the sensitivity of the samples to storage under dry nitrogen. The effect of exposure to air was investigated. The shape of the photoefficiency curves was found to agree quite well with that expected from the photoabsorption cross sections of the materials. CsI in particular appears useful as a detector in soft x-ray diagnostics, especially as a narrowband detector in the 100-eV photon energy range where peak measured efficiencies can exceed 300%.

There has been increased interest recently in time-resolved measurements of UV and soft x-ray emission for the study of picosecond processes in fusion plasmas, biological systems, atomic collisions, and photochemical reactions. High sensitivity x-ray photocathodes for use in diodes or streak cameras could enhance the capability of existing diagnostic equipment used in these research areas. Two high-sensitivity photocathode surfaces, CsI and CuI,¹ were evaluated and compared with an evaporated aluminum surface. Their efficiencies are substantially higher than aluminum (factors of 5-50 near 100-eV photon energy).

Several characteristics are important for a photocathode surface to be useful for ultrafast temporal diagnostics. These include good efficiency, reproducibility from batch to batch or good exposure and shelf-life characteristics, and a narrow secondary electron emission spectrum. In the results reported here, these characteristics are evaluated for CuI and CsI.

The electron emission of a photocathode involves several processes. Absorption of incident radiation leads to the generation of primary electrons. If the

material thickness is larger than the primary electron range, a number of lower energy secondary electrons are created by each primary. In addition, the atoms excited by the incident radiation decay through fluorescence and Auger processes creating additional electrons. A certain number of the secondary electrons reach the photocathode surface with enough energy to escape. These electrons are measurable as a photoemission current.

The photoemission is proportional to the incident photon energy, the photon absorption characteristics, and the material's electron properties. From a simple phenomenological model, the photoemission is proportional to $\rho p E \mu(E) f(E)$, where I is the incident x-ray intensity (photons/cm² sec), ρ is the mass density, E is the photon energy, $\mu(E)$ is the mass photoionization cross section, and $f(E)$ is the fraction of total energy deposited that is effective in secondary electron emission. This efficiency factor $f(E)$ is strongly material dependent. In metals, the predominant secondary electron generation mechanism is electron-electron collisions, while for semiconductors and insulators, where the number of free conduction electrons is lower, processes other than electron-electron collisions can be important. For example, in semiconductors (CuI), hole-pair formation plays an important role in creating low-energy electrons, while in insulators (CsI), electron-phonon processes (lattice vibration) can be significant. The dominance of different generation processes leads to widely varying values of secondary electron production efficiency, as will be seen.

The secondary electron generation process not only affects the emission efficiency but also the photoelectron energy distribution. Presented in Fig. 1 are the photoelectron energy distributions for the gold, aluminum (effectively Al₂O₃), copper iodide, and cesium

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Multilayer X-Ray Spectrometry in the 20–80 Region: A Molecular Orbital Analysis of CO and CO₂ in the Gas and Solid States

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Optimized multilayer X-ray spectrometry, using lead myristate and lead stearate analyzers (2d values of 80 and 100 Å) has been applied to the measurement of the O–K α and the C–K α spectral bands from CO and CO₂ in the gas and solid phases. The L_{II,III} spectra were also measured for argon in the gas and solid states under similar conditions in order to identify and to minimize any non-molecular components in the CO and CO₂ spectra. These molecular orbital data have been related to those obtained with X-ray and ultraviolet photoelectron spectroscopy and grating X-ray spectroscopy. The consistency of the results of these complementary measurements is excellent. The ionization energies for the C and O 1s levels have been determined to be 295.4 and 542.0 eV for CO and 296.8 and 540.3 eV for CO₂. The MO data have also been compared with that predicted from the symmetry, strength and binding energy of the molecular orbital spectral components as calculated using the currently available computational models, CNDO/2, MINDO/3, MNDO, extended Hückel and *ab initio*. The molecular orbital calculated results for these organic compounds, CO and CO₂, are not in as good agreement with the experimental data as previously demonstrated for molecular orbital spectra measured for C–K α and the L_{II,III} bands of Cl, S and P for both organic and inorganic compounds.

INTRODUCTION

A molecular group of atoms is chemically characterized by the symmetries, strengths and binding energies of the molecular orbitals that are generated from the valence electrons of the atoms involved. In recent years, with the increased availability of large computers, more accurate programs have been developed for calculating these molecular orbital characteristics.¹ Because the more efficient of these programs are semi-empirical at this time, it is of considerable value to have precise experimental molecular orbital data on a selected series of molecular systems as can be obtained with photoelectron and X-ray spectroscopy. The molecular orbital binding energies can usually be measured within 1 eV or better by ultraviolet (UPS) or X-ray (XPS) photoelectron spectroscopy. The X-ray spectrometry of the fluorescent radiation resulting from single electron transitions from the molecular orbitals into single ionization vacancies in the nearby, relatively sharp core levels can provide data on the symmetries and the relative strengths of the molecular orbital components as well. For example, the K α bands of the first-row elements reflect the p-character of the orbitals that are most strongly associated with the particular atom with the initial 1s vacancy. For the second-row elements, in a similar way, the K β bands and the L_{II,III} bands measure the p-character and the s- and d-character, respectively, of the associated molecular orbitals. These K β and L_{II,III} radiations are mostly in the 20–100 Å wavelength region. X-ray spectrometry in this long wavelength region requires either grating incidence diffraction gratings or large d-spacing multilayer analyzers.

In order to generate the 'cleanest' spectra possible that are characteristic of the simple, single-electron transitions (and therefore which can be directly and quantitatively related to the calculated molecular orbital symmetries, populations and binding energies), it is necessary to minimize and to identify extraneous spectral features. For example, effects resulting from multiple ionization, high-order diffraction and radiation damage must be minimized. This can be accomplished by using photon excitation so as to selectively excite the desired initial core level vacancy. But even with such selective deposition of the excitation energy, the total spectral energy that is allowed for measurement is often seriously limited by the requirement that the excitation damage should not cause significant radiation-induced changes in the sample. In order to meet the requirement for 'fast' X-ray spectroscopy, an optimized, high-efficiency spectroscopy has been developed^{2,3} which utilizes multilayer analyzers such as the lead myristate, lead stearate and lead lignocerate systems with 2d-spacings of about 80, 100 and 130 Å, respectively. Because the transmission functions of the multilayer spectrograph can be accurately measured, the attainable energy resolution can be in the sub-electron-volt region through simple spectral deconvolution procedures.

Multilayer measurements of the L_{II,III} spectral bands for the second-row elements, Cl, S and P, have been reported from this laboratory^{4–6} as applied to the molecular orbital analyses of a selected series of chlorine, sulfur and phosphorus compounds. The samples were polycrystalline and it was established that the molecular orbital spectra for the central atoms of the anions were not affected significantly by crystal field effects (different cations). More recently, C–K α and Cl–L_{II,III} spectral band measurements by multilayer X-ray spectrometry have been applied to the

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X-RAY SPECTROSCOPY IN THE 100-1000 eV REGION

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Some current methods for achieving low energy X-ray spectroscopy in the 10-100 Å region are reviewed. Gratings, crystals and multilayers can be used as monochromators or dispersive analyzers. Some of the important characteristics are noted here which can help to determine their applicability to a given spectroscopic analysis situation. The "trade-off" between resolution and spectrographic speed (gratings versus multilayers) may be an important consideration when the number of photons available for measurement is limited, as, for example, by the excitation dosage allowed for a given sample. For pulsed X-ray sources and for time-resolved spectroscopy, special fixed-crystal spectrographs have been developed. These may be applied with X-ray diodes and fast oscilloscopes or with X-ray streak cameras for detection. The optimum design and characterization of the photocathode systems for such detection have been studied in detail and some of the results of this work are briefly reviewed.

1. Introduction

The new synchrotron radiation and laser-produced plasma sources can provide pulsed, broad-band radiation in the UV and X-ray region of such high intensity as to present a new dimension for spectroscopic analysis. This may be of particular importance for low energy X-ray spectroscopy in the 10-100 Å region for which high intensity, selective excitation has generally not been available.

X-ray absorption and emission spectroscopy in this low energy region is of considerable interest for the measurement of the spectra that originate from transitions between the outermost electronic levels and the relatively sharp, first core levels. Such valence band spectroscopy can sensitively reflect the chemical, optical and electronic properties of matter.

The importance of having continuous selectivity of the excitation for absorption spectrometry is well known, particularly for extended absorption fine structure measurements. Selective, narrow-band excitation can also present a critical advantage in emission spectrometry by providing "clean" meaningful spectra with a minimum of background radiation, and by minimizing possible effects of radiation-induced changes in the sample.

An illustration of the critical role of radiation damage in molecular orbital spectroscopy is presented in fig. 1. The chlorine-L_{II,III} spectra in the 150-250 eV region were measured in order to determine the relative molecular orbital strengths of s and d symmetries for various oxidation states in chlorine

Fig. 1. Radiation-induced decomposition of polycrystalline NaClO_4 . The excitation intensity was similar to that employed for the Cl-L_{II,III} spectroscopy [1.75×10^{13} C-K α (277 eV) photons/s cm^2 at the sample surface]. The quick scans reveal spectral changes corresponding to the appearance of reduction products such as NaClO_3 and NaClO_2 . After three hours, the spectra correspond to that for NaCl.

The characterization of x-ray photocathodes in the 0.1–10-keV photon energy region

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A method and an instrument are described for the measurement of the absolute quantum yield for front-surface and transmission photocathodes in the 0.1–10-keV photon energy region. The total and the secondary electron photoemission yields have been measured for the Al, Au, CuI, and CsI photocathodes as required for the absolute calibration of the x-ray diode detectors and for the x-ray streak cameras. The relative secondary electron yields have also been measured for the same photocathodes by high resolution electron spectroscopy of the secondary electron energy distributions, which are in good agreement with the absolute yield measurements. The secondary electron yield of CsI is ten to one-hundred times higher than that for Au in the 0.1–10-keV region and with a secondary energy distribution that is appreciably sharper. For these reasons, CsI should be an effective photocathode for sensitive, time-resolved spectroscopy into the picosecond region. It is verified experimentally that the secondary electron quantum yield varies approximately as $E\mu(E)$, with E as the photon energy and $\mu(E)$ as the photoionization cross section, and that the primary (fast) electron quantum yield is a small fraction of the total yield and varies approximately as $E^2\mu(E)$. A simple model for x-ray photoemission is described which leads to semiempirical equations for front- and back-surface secondary electron photoemission as based upon an escape depth parameter that may be obtained from yield-versus-photocathode thickness data. The model predictions are in good agreement with experiment.

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I. INTRODUCTION

Time-resolved x-ray spectroscopy has become of considerable importance in the temperature density composition diagnostics of high-temperature plasmas involved in controlled thermonuclear fusion studies which utilize laser, particle beam, or magnetic compression-confinement production. The time duration of the associated x-ray emission ranges from picoseconds to seconds. Time-resolved x-ray spectroscopy is also important in the development of super-radiant, pulsed x-ray sources, their application to studies of the radiation effects of x-ray bursts upon materials, and the x-ray analysis of atomic, molecular, and solid-state time-resolved processes into the picosecond region.

The electron currents that are emitted by photocathodes under x-ray excitation can be a very effective basis for time resolved spectroscopic measurement using x-ray diode or streak camera detection.^{1–5} In the latter, an x-ray spectrum can be established along a slit-defined transmission photocathode of the streak camera by using focussing filter-total-reflection monochromator, crystal/multilayer arrays, or nonfocussing, Bragg reflecting crystal/multilayer analyzer systems.

In time-resolved x-ray spectroscopy, the ultimate limit on the achievable time resolution is the quantum conversion efficiency of the photocathode (which determines signal statistics) and the energy spread of the emitted electrons as is noted in Fig. 1 (which determines the time resolution).⁶ The relatively small fraction of fast electrons that is photoemitted is effectively blocked by the electron optical apertures of

the typical streak camera. In Fig. 2 the difference in the arrival time at the output end of the streak camera is given as a function of the energy width Δ of the secondary electron energy distribution, the extraction field ϵ_0 , and of the geometry of the camera. In addition to the absolute yield-versus-photon energy and the shape of the secondary electron distribution curves, other important characteristics of the x-ray photocathode are its stability, reproducibility, simplicity of spectral response, and the linearity of its time response. Described here is a method and an instrument for the measurement of the absolute total and secondary electron yields

FIG. 1. In the 0.1–10-keV photon energy region the larger fraction of the electrons that are emitted are the secondary electrons, typically as a narrow distribution below 10 eV. The higher energy, fast electron photoemission consists of relatively sharp elastically scattered photoelectrons and Auger electron "lines" along with a much larger number of inelastically scattered electrons in their low-energy tail region.

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X-RAY DIFFRACTION IN MULTILAYERS

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Diffraction of X-rays in multilayer systems such as the molecular and the evaporated/sputtered multi-layers have been studied based upon the optics of thin films. General solutions for the intensity profiles of x-ray diffraction from multi-layers of finite thickness have been obtained for angles of incidence outside the total reflection region. It is also shown that the optical expression for diffraction in the x-ray region by periodic systems agree with the conventional crystal diffraction theories.

1. Introduction

Improved experimental techniques have generated considerable interest in the application of evaporated [1] and sputtered [2] multilayers (ESM) as analyzers and monochromators in the ultrasoft x-ray region (10–100 Å). Variable film thicknesses and materials enable ESM to operate in regions between acid phthalate crystals and the molecular multilayers such as the Langmuir-Blodgett systems.

For crystals, there are two principle theories which may be invoked to account for the intensities observed in x-ray diffraction studies. The kinematical theory assumes that there is no appreciable absorption or multiple reflection of radiation in the crystal medium and hence is valid only for extremely thin crystals. Dynamical theory, on the other hand, takes into account all wave interactions within the crystal, and must be used whenever diffraction by large perfect crystals is of interest. As a general rule, if the thickness of the diffraction region and the reflection per plane are sufficiently small that multiple interplay of beams is negligible, then the results predicted by the dynamical diffraction formulae (i.e., Darwin-Prins or Ewald models) approach those predicted by the kinematical formula [3–5].

The calculated intensities of x-ray diffraction from ESM have been based upon the optics of thin films. This approach is the summation of all the reflection and refraction fields of x-rays at the plane interface of two adjacent media of different index of refraction, n . Numerous authors have given expressions for the intensity ratio of the incident beam to the reflected beam of a finite number of films in terms of recursion formulae [6–8]. Recently the peak reflectivity for ESM with two films per period has been obtained in closed form [9].

It is the intention of this communication to extend the theory of x-ray diffraction by ESM and to unify the crystal x-ray diffraction theory with the theory of interference films. Sect. 2.1 considers the case of N periodic multilayers with two films per period. Expressions for the profile of the diffracted beam has been derived in closed form for all angles of incidence outside the total reflection region. Sect. 2.2 deals with the general case of s layers per period. Sect. 3 generalizes the formalism developed in the previous section to the case of x-ray diffraction by crystals. Diffraction formulae valid for arbitrary number of layers are given. The final sect. 4 gives a comparison for various N , of the calculated diffraction profiles for a few of the crystals and multilayers of current interest.

Considerable algebraic simplification in the x-ray region results from the refractive index, n , being nearly

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The Stability of Cesium Iodide X-Ray Photocathodes

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ABSTRACT

For pulsed x-ray measurements as applied, for example, in high temperature plasma diagnostics, it has been recently established that the cesium iodide photocathode is very efficient in x-ray diode (XPD) and streak camera applications. Its quantum yield (electrons/photon) is ten to one-hundred times higher than that for the gold photocathode in the 100-10,000 eV region. The width of its secondary electron energy distribution is appreciably smaller than that for gold, allowing time resolved, streak camera measurements to be extended into the picosecond region. In this note, an experimental study is described which has demonstrated that the cesium iodide photocathode quantum yield and secondary electron energy distribution characteristics can be very stable under practical conditions of preparation, handling, storage and short period exposures to the atmosphere.

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