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TITLE CALIBRATIONS OF A MULTICHANNEL SOFT X-RAY SPECTROMETER

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Calibrations of a multichannel soft x-ray spectrometer

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Abstract

A time resolved, 14 channel spectrometer with an absolutely calibrated response, was developed to cover an x-ray photon energy spectrum from 70 to 650 eV. The spectrometer utilized a combination of thin film prefilters, layered synthetic microstructure (LSM) diffractors, metal coated plastic scintillators, and photomultiplier detector tubes. Calibration of the spectrometer was done piecemeal for each component with standard techniques and the component calibrations were convolved to get a complete spectrometer response function. The complete assembled system was also calibrated at a synchrotron beamline. The two calibration procedures were compared.

Introduction

Recently, Los Alamos National Laboratory (LANL) has become involved in using layered synthetic microstructures (LSM) in spectrometers for plasma diagnostics. The ability to control the structure of the LSM and, therefore, the dispersion properties for channel energy response definition, has been the major reason for their development. In this paper we will describe the design and calibration of a multichannel LSM spectrometer.

The goal of the spectrometer was to obtain via a remote oscilloscope an absolute intensity spectra with a 250 megahertz bandwidth from a plasma at a blackbody temperature of 70 eV. The plan was to use LSM Bragg diffraction to define 10 distinct energy channels (slices) of the assumed blackbody spectrum as shown in Figure 1.

Figure 1. The spectrometer's designed spectral response.

Spectrometer design

With the spectrometer goal in mind, the first step in designing the spectrometer was to employ a matrix method of solving the EMM boundary conditions at each interface¹ (OEM model) to predict the reflectivity properties of LSMs. The model was coded on a computer and several iterations were run for each channel with the goal of minimizing the low energy total reflection effects, reducing the higher order diffraction, and choosing predictable material combinations. For these reasons two Bragg angles were chosen: 60 degrees for the low-energy set and 22.5 degrees for the high-energy set as shown in Figure 2. The low-energy set has a narrower energy response width and reduced integrated reflectivity, while the 22.5 degree Bragg angle set compensated for the reduced spectral intensity in the high-energy tail of the source spectrum by increasing the integrated reflectivity. Both sets required filters to help eliminate the specular reflection component. Calculations showed that one could reduce the specular reflection component by choosing the lighter element which has a small f_1 value near the channel energy for the top layer. In addition, the thickness fraction of heavy material was chosen to be .5 to eliminate even diffraction orders. The following material combinations with their respective energy ranges were chosen for the spectrometer: Mo/Si 70-100 eV, Pd/B4C 100-180 eV, V/C 100-350 eV, W/C 450-650 eV.

After the LSM sets were determined, the detectors and filters were chosen, as shown in the schematic drawing of Figure 3. Plastic BC422 scintillators with photomultiplier tubes were chosen because they could be packed into a tight geometry required by the experiment. The high sensitivity of the PM tubes allowed for thick filters, thus reducing the heat load on the LSMs. The maximum surface temperature rise expected during the period of interest was calculated to be 700°C for the channel 2 Mo/Si LSM with a carbon prefilter. A more typical temperature rise was 40°C on channel 1 Mo/Si LSM with a 1.4 μm Al prefilter. The prefilters were also used to adjust the signal level. The last filters in the system were the 2000 Å aluminum or titanium metal coatings on the scintillators. These were to act as visible light blocking filters.

Figure 2. A schematic diagram of the spectrometer's geometry.

Figure 3. A schematic diagram of the spectrometer's response defining components.

Calibration of the spectrometer

The calibration of the spectrometer was done by first calibrating each of the components and second by calibrating the total system on the LANL VUV beamline at the National Synchrotron Light Source (NSLS) at the Brookhaven National Laboratory. The component calibrations were done at the following facilities:

<u>Component</u>	<u>Facility, measurement, and contact</u>
LSM	Ovonic Synthetic Materials Co., a division of Energy Conversion Devices (ECD) Reflectivities and d-spacings at Cu-K wavelength James Wood
LSM	Lawrence Berkeley Laboratory Reflectivities, rocking curve widths, and d-spacings at C-K, Cu-L, and Al-K wavelengths Burton Henke
LSM	Los Alamos National Laboratory Rocking curves at Cu-L John Grosso
Prefilters	Los Alamos National Laboratory Filter transmissions at C-K, Mg-K, and Al-K Joe Chmielewski
Scintillator and photomultiplier tubes	EG&G Energy Measurements Group Calibrations at C-K, O-K, F-K, Ni-L, Mg-K, and Al-K Ping Po Gong and Leif Singman

Spectrometric properties of the LSMs

The principal reason for accurately determining diffraction characteristics of the LSMs at the laboratory wavelengths was to have benchmarks to determine the physical characteristics of the LSMs. This enabled us to use the OEM model to predict the LSMs' total performance. These predictions would also provide a check of the spectrometer's calibration on the synchrotron system.

The three LSM calibrations were done by three different methods. The first measurement, done by ECD, was to check each LSM d-spacing after each was sputtered at ECD. The measurement was done by using a filtered and collimated Cu-K line source from an x-ray tube to produce diffraction peaks up to the 19th order in the case of a 100 Å d-spacing. To find the true d-spacing the OEM model was used to compute the index of refraction correction. Measured peak angle differences between the various orders were used with the computed index of refraction at Cu-K to determine the diffractometer zero error and the true d-spacing. The d-spacing results are displayed in Table 1.

The second measurement was done at Lawrence Berkeley Laboratory (LBL). The rocking curves were estimated from measurements taken with collimated Henke tubes at the characteristic x-ray lines of C-K, Cu-L, and Al-K. The zero angle was determined from low angle reflectivity cutoff and two or more diffraction orders were measured. The true d-spacing was determined by plotting the effective d-spacing vs. $\csc^2(\theta)$ as described by Henke.² The FWHM and the peak reflectivity were obtained by matching a modified Darwin-Prins model,² folded with the estimated collimator width and line width to the data. The results are displayed in Table 1 and Table 2.

The third set of spectrometric properties was measured at LANL by using a Cu-L-line source and a two crystal instrument with appropriate apertures and a potassium acid phthalate (KAP) first crystal. The double crystal rocking curve of two halves of a cleaved KAP crystal was measured at Al-K. This showed the single crystal rocking curve of one of the KAP crystals was near theoretical at Al-K α , so we could calculate its value to be 1.1 arc min at Cu-L.¹ Thus, since the pre-crystal function was less than 1/16 the narrowest LSM rocking curve width, the effect was treated as an uncertainty limit of the rocking curves. Separate measurements of the direct beam, I_0 , were made. The peak reflectivity and FWHM were directly determined from the data. The true d-spacing was determined by adjusting the d-spacing in the OEM model to match the predicted 1st order peak angle to the measured value. Results are presented in Table 1 and Table 2. Comparison of the three measurements shows that there is good agreement between the ECD d-spacing and the LBL d-spacing, while the

d-spacing required in the OEM model to match the LANL first order Cu-L peak was consistently lower. In order to use the rocking curve measurements at laboratory wavelengths to estimate the response of the spectrometer at the wavelengths of each channel, the simplest adjustment to the OEM model was to assume that the reduced reflectivity is due to a gaussian distribution of the uncertainty in the d-spacing to account for roughness at the layer interfaces. The peak reflectivity is then reduced by a "Debye-Waller" like factor that assumes an interfacial roughness and is calculated by the following formula.

$$\eta = \frac{P(\text{measured})}{P(\text{calculated})} = \exp \left[-\left(\frac{2\pi n \Delta Z}{d} \right)^2 \right]$$

Where n is the diffraction order, ΔZ is the RMS interface roughness, P is the peak reflectivity, and d is the distance between the scattering layers.

Comparisons of the OEM model with the "Debye-Waller" like factor to the LANL rocking curve measurements are presented for four representative LSM samples in Figures 4-7.

Figure 4. Comparison of the channel 1 Mo/Si LSM rocking curve data to the OEM model.

Figure 5. Comparison of the channel 2 Mo/Si LSM rocking curve data to the OEM model.

Figure 6. Comparison of the channel 8 C/V LSM rocking curve data to the OEM model.

Figure 7. Comparison of the channel 12 C/W LSM rocking curve data to the OEM model.

Prefilter transmission measurements

Prefilter transmission measurements were done by translating the filters in and out of a collimated x-ray beam whose intensity was measured by a proportional counter. Mg-K and Al-K x-rays were produced with fluorescent targets and C-K x-rays were produced with a Carbon anode x-ray tube.

Scintillator and photomultiplier tube calibrations

These measurements were done by using collimated characteristic x-ray lines from fluorescent targets or directly from a filtered Henke-tube source. An x-ray beam was defined by aperture plates to be within the active area of the scintillator and the entire scintillator-light-pipe-photomultiplier-tube-detector stack was translated to move into the beam detector by detector. Each photomultiplier tube was separately measured for its visible light response at the scintillator wavelength and its electronic characteristics were optimized.

Synchrotron measurements

The assembled spectrometer without the pre-filters was connected via an EG&G vacuum interface to the LANL synchrotron beamline. It should be noted that this was the first operational use of the LANL beamline.

The LANL synchrotron low energy beamline basically consisted of an "Extended Range Grasshopper" which provided a monochromator beam with the following characteristics:

<u>Energy range</u>	<u>Resolving Power</u>	<u>Beam Uniformity</u>	<u>Polarization</u>
20 - 1000 eV	$E/\Delta E \sim 100$	Inhomogeneous	Horizontal

The calibration consisted of positioning the spectrometer to have the "monochromatic" x-ray beam incident on one channel at a time, scanning the beam in energy (while monitoring the beam intensity with an aluminized transmission mesh photocathode), and measuring the current output of the photomultiplier tubes with an electrometer. When the scan was completed, the aluminized mesh beam monitor was cross calibrated to an NBS x-ray diode through an unoccupied position in the LSM array. The NBS diode has since been post calibrated at the NBS synchrotron facility to $\sim 10\%$ accuracy over the energy range of 10 to 250 eV. Because the LANL beamline was being used for the first time, many idiosyncrasies had not been resolved. For example, the beam inhomogeneity varied with time, higher orders were present in the spectral beam and stray light was high from at least one grating. Therefore, the absolute flux calibrations were poorly determined. However, the shapes of the response functions for all channels were reasonably measured. It was also necessary to shift the synchrotron response curves in energy to match the channel energies estimated from d-spacings.

It was discovered during calibration that the intensity of the monochromated beam was lower than expected. With the low gain of 1000 of the photomultiplier tubes this produced a signal that was comparable to the dark current signal of many of the photomultiplier tubes. Therefore, we selected the photomultiplier tube with lowest dark current and interchanged it from one channel to another for the calibrations. Also, the prefilter set was not included in the synchrotron calibration as originally planned, but was measured adequately as noted earlier.

Using the d-spacing determined from the laboratory LSM data, a comparison of the OEM model could be made to the synchrotron data, provided that one accounts for the metal coated scintillator response which is included in the measured synchrotron spectrometer response. The first comparison is shown in Figure 8, with the synchrotron data arbitrarily scaled to the LANL laboratory reflectivity curve. This lowest energy channel was targeted to be below the Al-L edge. As can be seen from the synchrotron data, the Al-L edge from the scintillator coating appears to be centered on the channel response. This edge effect does not appear on the calculated response curve because the Al coated scintillator was not included in the OEM model. This comparison shows dramatically how important the synchrotron beamline can be simply to reveal the inadequacies of calibration by piecemeal measurement and extrapolation. The next step was to compare the calibrations on channels where the coated scintillator response was expected to be relatively flat. In Figure 9 and Figure 10 the synchrotron data were shifted and scaled to match the peak and the wings of the model. As can be seen, the shape of the data matches the prediction within the error bars. The third comparison was for channel 2, shown in Figure 11, with the synchrotron data scaled to the peak of the OEM model. Here the OEM model predicted a non-symmetrical curve compared to the synchrotron data. Additional measurements done at the synchrotron included measurement of cross-talk between neighboring channels. This was found to be significant and will be included in the total detector response.

Figure 8. Comparison of the channel 1 Mo/Si OEM model to the synchrotron data. The data has been vertically scaled to appear on the reflectivity plot and the energy scale shifted to the 72.78 eV Al-L₃ edge.

Figure 9. Comparison of the channel 8 C/V OEM model to the synchrotron data. The data has been vertically scaled to match the peak of the model and the energy scale has been shifted to match the peak of the model.

Figure 10. Comparison of the channel 12 C/W OEM model to the synchrotron data. The data has been vertically scaled to match the peak of the model and the energy scale has been shifted to match the peak of the model.

Figure 11. Comparison of the channel 2 Mo/Si OEM model to the synchrotron data. The data has been vertically scaled to match the peak of the model. The energy scale has been calibrated using the 72.78 Al-L₃ edge.

Discussion

In general, the calculated rocking curves are expected to show narrower widths and lower tails than measured rocking curves. This is because the measurements have a small instrument function that has not been deconvolved and measurements include some lower energy "impurity" radiation that can specularly reflect. Both effects are small for our systems. Therefore, we feel justified in making adjustments to the OEM model parameters, especially Γ and layer roughness. From continued work on modeling these samples to match the observations, we hope to gain some insight on the distinction between surface roughness and diffusion at layer boundaries. In the comparison of the OEM model to the Mo/Si LSMs used in channel 1 and 2, the model was unable to fit all the observed features in the data. The largest discrepancy was in the energy width of the channel 2 LSM reflection shown in Figure 11. The proposed explanation is that the actual LSMs are made up of intermixed layers, and not distinct homogeneous layers as assumed for these cases. The OEM model has the capability of calculating roughness and a full range of layer mixing layer by layer. The goal of future modeling is to fit the full rocking curves from the low angle specular reflection region to the highest orders in order to fully define the LSM parameters. Meanwhile, we are gratified to be able to make a single wavelength rocking curve measurement, adjust the OEM model parameters to fit the data, re-calculate the rocking curve at a far different wavelength, and get reasonable agreement with synchrotron measured response functions, as with channels 8 and 12.

Earlier, we remarked on the systematically lower values of 2d-spacing derived from OEM model fits to the LANL measurements than from LBL or ECD measurements (Table 1). In fact, measurements were not made on identical LSM pieces. ECD measured some wafers before shipment to LANL. At LANL the central portion was taken out for the experiment and an adjacent piece was forwarded to LBL. This does not explain the measured differences because, (1) LANL had measurements across the full three inch diameter of one wafer that agreed within 2.5% across the wafer, (2) the pieces measured by LBL would show less deviation than this because they were adjacent to the center piece, (3) the ECD and LBL results agreed within 2% (four out of five were within 1%), and (4) the discrepancy of the LANL results compared to the others varied from 1% to 11%. Where possible, we have used the LBL or ECD values. Since the LANL data lacked multiple order reflections it was not possible to extrapolate the true d-spacing. Rather, we had to use the OEM model to estimate the corrections for dispersion at 13.3 Å. The discrepancies might be reduced some by varying Γ , layer mixing, and layer roughness parameters in the OEM model.

A different situation exists with rocking curve widths in Table 2. The LANL values vary from 17% smaller to 40% larger than LBL values, all measured at the same wavelength. These differences are, no doubt, real since they exceed about 10%. Recall that measurements were made on adjacent pieces from the same wafer. Peak reflectivities show even larger discrepancies. Here we tend to rely more on LANL values because the rocking curves are directly measured. The need to scale down the calculated values to match observations is a persistent feature that has characterized most LSM samples to date. It appears consistently in the last column of Table 2. These combined measurements show that existing production controls are not yet adequate to consistently provide LSM samples whose spectrometric properties are predictable to better than 50%, whether on peak reflectivities, rocking curve widths, or integrated reflection coefficients. In all probability, layer roughness and interlayer diffusion are not the only relevant variables, as evidenced by the wide variation in spectrometric properties of adjacent samples from the same wafers (LBL vs. LANL measurements).

Conclusions

Our calibration tasks are not yet complete. Data shown in this report demonstrate that we still need to make LSM measurements at LANL on the exact same pieces that were measured at LBL. Hopefully, that will indicate which production variables must be controlled more carefully. Meanwhile, the spectrometric properties measured at LANL will be used for calibrations of the entire spectrometer. Data reductions and further detailed modeling will then be done. At this point, the ability to extrapolate results from one wavelength to another is not sufficient for accuracies better than 50%. The importance of a well characterized synchrotron beam for calibration accuracies (~ 10%) cannot be overemphasized.

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Table 1. Comparison of d-spacing determinations

Spectrometer Channel No.	Material Combination		Effective d-spacing measured by ECD at $\lambda=1.54\text{\AA}$ (A)	Effective d-spacing measured by LANL at $\lambda=13.336\text{\AA}$ 1st Order (A)	d_{α} determined by LBL at $\lambda=13.336\text{\AA}$ (A)	d_{ω} determined by ECD/OEM at $\lambda=1.54\text{\AA}$ (A)	d-spacing used in OEM model to match LANL 1st order $\lambda=13.336\text{\AA}$	Used in the OEM model
	top layer/ bottom layer	No. of layer pairs						
1	Mo/Si	60	102.25 $\pm$ 1.8	85.10 $\pm$ 2.1	105.10 $\pm$.45 104.14 $\pm$.45 ^b	106.29 $\pm$.40	100.94	.5
2	Mo/Si	95	73.80 $\pm$ 1.2	70.86 $\pm$ 1.7	82.49 $\pm$.35 84.33 $\pm$.35 ^c	82.50 $\pm$.31	76.57	.395
3	C/V	50	51.15 $\pm$ 1.1	49.37 $\pm$ 1.2	53.14 $\pm$.23		47.70	.5
4	C/V	60	39.70 $\pm$.37	37.66 $\pm$.92	40.33 $\pm$.17		38.72	.5
5	C/V	90	31.13 $\pm$.71	31.10 $\pm$.76			31.64	.5
6	C/V	100	26.03 $\pm$.25	25.41 $\pm$.62			25.73	.5
8	C/V	50	70.43 $\pm$.87	66.26 $\pm$ 1.6	75.15 $\pm$.32		72.04	.5
9	C/V	52	58.90 $\pm$.57	54.63 $\pm$ 1.3	58.21 $\pm$.25		57.80	.5
10	C/V	60	46.29 $\pm$.46	44.24 $\pm$ 1.1	48.25 $\pm$.21		45.87	.5
11	C/W	60	36.00 $\pm$.28	35.36 $\pm$.87	37.61 $\pm$.15	37.77 $\pm$.14	36.56	.5
12	C/W	75	29.46 $\pm$.21	28.62 $\pm$.70 ^a	30.29 $\pm$.13	30.09 $\pm$.11	29.35	.5
13	W/C	90	24.92 $\pm$.24	24.05 $\pm$.6	25.61 $\pm$.1 25.70 $\pm$.1 ^b	26.13 $\pm$.10	24.43	.5

^a The uncertainty in measuring four samples across the silicon wafer sample

^b Measured at Al-K α x-rays $\lambda = 8.34\text{\AA}$

^c Measured at C-K x-rays $\lambda = 44.7\text{\AA}$

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Spectrometer Channel		FWHM measured by LANL at 929.7 eV (mr)	FWHM determined by LBL at 929.7 eV (mr)	FWHM predicted by OEM model at 929.7 eV (mr)	Peak reflectivity measured by LANL at 929.7 eV	Peak reflectivity determined by LBL at 929.7 eV	Peak reflectivity predicted by the OEM model	η LANL peak measurements divided by the OEM model
No.	Material							
1	Mo/Si	11.4 $\pm$.22 .27	10.20	10.0	.166 $\pm$.0015	.2125	.3416	.482
2	Mo/Si	10.6 $\pm$.22 .27	10.25	8.19	.176 $\pm$.0015	.1375	.3904	.441
3	C/V	6.1 $\pm$.22 .27	6.31	4.46	.0614 $\pm$.0010	.0265	.1653	.371
4	C/V	6.1 $\pm$.22 .27		4.02	.0615 $\pm$.0009		.16	.384
5	C/V	5.3 $\pm$.22 .27		3.49	.0573 $\pm$.0009		.1554	.369
6	C/V	5.7 $\pm$.22 .27		3.07	.0440 $\pm$.0008		.1460	.301
8	C/V	7.0 $\pm$.22 .27	8.4	5.86	.0556 $\pm$.0008	.0368	.16	.348
9	C/V	6.9 $\pm$.22 .27	6.59	5.75	.0849 $\pm$.0008	.0549	.163	.521
10	C/V	5.7 $\pm$.22 .27	5.23	4.21	.0597 $\pm$.0010	.0644	.1664	.359
11	C/W	8.7 $\pm$.22 .27	6.19	6.69	.152 $\pm$.0015	.1149	.5264	.289
12	C/W	7.0 $\pm$.22 .27	5.92	5.76	.148 $\pm$.0014	.1146	.2398	.602
13	W/C	6.2 $\pm$.22 .27	4.77	5.07	.130 $\pm$.0014	.1199	.2597	.501

^a The FWHM determined at the half height of the peak minus the specular reflection component

^b The peak reflectivity including the specular reflection component