Introduction to Grating Analysis

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Acknowledgements: Randall Smith, Dave Huenemoerder

See also David Huenemoerder’s spectroscopy page
http://space.mit.edu/ASC/analysis/AGfCHRS/AGfCHRS.html
Chandra has two transmission grating spectrometers.

The LETG: Spacing = 1\(\mu\)m

\[
\text{FWHM} = .05 \text{ Å}
\]

The HETG: Spacing = 0.2, 0.4 \(\mu\)m

\[
\text{FWHM} = .012, .024 \text{ Å}
\]
Either one of the two grating assemblies can be inserted at any time:

The gratings and the detectors are entirely independent, and so any combination may be selected (although some are less useful than others). The most common combinations are:

• HETG/ACIS-S
• LETG/ACIS-S
• LETG/HRC-S
Capella with the HETG/ACIS-S detector:

Spectrum from the MEG-1 order
High-resolution (grating) spectra on Chandra cover a wide range of wavelengths: from 1.2-170Å. Note that wavelength is the natural unit.

LETG/HRC-S Observation of NGC6624

Grating Basics

X-ray gratings work exactly the same as optical gratings: the photons hit the gratings, and some are dispersed in a wavelength-dependent fashion, following the grating equation: \[ \sin \beta = m \frac{\lambda}{p} \]

where \( \lambda \) is the wavelength, \( \beta \) is the dispersion angle (measured from the zero-order image), \( p \) is the spatial period of the grating lines, and \( m \) is the order number.
If ACIS is the detector, the CCD resolution can be used to distinguish between different orders; on the HRC, order separation must be modeled.

The goal of the grating pipeline is to:

- Select “good” X-ray events
- Identify the zero order and dispersed image
- Measure the dispersion angle for each event
- Create a binned spectrum
- Calculate the effective area and response matrix

Clearly, the spatial and spectral elements are tightly coupled. If the zero-order image is slightly displaced, the ± order wavelengths will be offset from each other.

Note: By default, pixel randomization is turned “on” in the *_process_events step. If you are not concerned about timing fluctuations on 1 ksec timescales, turning it off can increase the HEG resolution by 10%.
Identify zero-order, grating arms

tgdetect infile=hrc_evt1.fits outfile=hrc_evt1_src1a.fits OBJ_srclist_file=NULL

Make mask for each grating arm (tg_create_mask)

tg_create_mask infile=frc_evt1.fits outfile=hrc_evt_L1a.fits

input_pos_tab=hrc_evt1_src1a.fits grating_obs=header_value

Measure dispersion angle for each event

tg_resolve_events infile=hrc_evt1.fits outfile=hrc_evt1a.fits regionfile=hrc_evt1_L1a.fits

acaofffile=hrc_aoff1.fits eventdef=")stdlev_HRC"

Apply background filter (dmcopy)

dmcopy "hrc_evt1.fits[EVENTS][pha=0:254, (tg_lam, pi)=region($CALDB/data/chandra/

hrc/bcf/tgmask2/letgD1999-07-22pireg062_N0001.fits])" hrc_back_evt1a.fits opt=all

Apply GTI filter (dmcopy) dmcopy "hrc_back_evt1a.fits[EVENTS][@hrc_std_flt1.fits][cols

!crsu,!crsv,!amp,!av1,!av2,!av3,!raw,!sumamps]" hrc_flt1_evt1a.fits opt=all

Filter on status (dmcopy)

dmcopy "hrc_flt1_evt1a.fits[status=xxxxxx00xxxx0xxx0000x000x00000xx]" hrc_evt2.fits opt=all

Extract a Grating Spectrum (tgextract)

tgextract infile=hrc_evt2.fits outfile=hrc_pha2.fits inregion_file=CALDB

outfile_type=pha_typeII tg_srcid_list=all tg_part_list=header_value tg_order_list=default

ancrfile=none respfile=none

Make grating effective area

fullgarf phafile=hrc_pha2.fits pharow=1 evtfile=hrc_evt2.fits asol=pcad_asol1.fits

engrid="hrc_rmf.fits[cols ENERG_LO,ENERG_HI]" dtffile=hrc_dtf1.fits

badpix=hrc_bpix1.fits rootname=x_per
The standard output is a single PHA file (Type II PHA), containing

**ACIS/HETG** 12 spectra (±1, 2, 3 orders for both the HEG and MEG).

**ACIS/LETG** 6 spectra (±1, 2, 3 orders for the LEG).

**HRC/LETG** 2 spectra are created (± orders).

**HRC/HETG** Not a recommended configuration

This “PHA2” is a FITS format file that contains N rows of data, one for each spectral order. The file can be viewed with **prism**. Other standard FITS output files are the grating arf (“garf”) and grating rmf (“grmf”).

The pha spectrum is in counts vs bin edges; dividing by the effective area (garf) and exposure time creates a fluxed spectrum. The instrumental line profile is essentially the grmf.

In Sherpa, grating spectra can be jointly fit to a model.
unix% dmfile hrc_evt2.fits cols

## Columns for Table Block EVENTS

<table>
<thead>
<tr>
<th>Col</th>
<th>Name</th>
<th>Unit</th>
<th>Type</th>
<th>Range</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>time</td>
<td>s</td>
<td>Real8</td>
<td>6.9e7:7.0e7</td>
<td>time tag of data record</td>
</tr>
<tr>
<td>2</td>
<td>rd(tg_r,tg_d)</td>
<td>deg</td>
<td>Real4</td>
<td>-2.0: 2.0</td>
<td>Grating angular coords</td>
</tr>
<tr>
<td>3</td>
<td>chip (chipx,chipy)</td>
<td>pixel</td>
<td>Int2</td>
<td>1:4096</td>
<td>Chip coords</td>
</tr>
<tr>
<td>4</td>
<td>tdet(tdetx,tdety)</td>
<td>pixel</td>
<td>Int4</td>
<td>1:49368</td>
<td>Tdet coords</td>
</tr>
<tr>
<td>5</td>
<td>det(detx,dety)</td>
<td>pixel</td>
<td>Real4</td>
<td>0.50:65536.50</td>
<td>Det coords</td>
</tr>
<tr>
<td>6</td>
<td>sky(x,y)</td>
<td>pixel</td>
<td>Real4</td>
<td>0.50:65536.50</td>
<td>Sky coords</td>
</tr>
<tr>
<td>7</td>
<td>chip_id</td>
<td>Int2</td>
<td></td>
<td>1:3</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>pha</td>
<td>Int2</td>
<td></td>
<td>0:255</td>
<td></td>
</tr>
<tr>
<td>9</td>
<td>pi</td>
<td>Int2</td>
<td></td>
<td>0:255</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>tg_m</td>
<td>Int2</td>
<td></td>
<td>-62:62</td>
<td>Diffraction order (m)</td>
</tr>
<tr>
<td>11</td>
<td>tg_lam</td>
<td>angstrom</td>
<td>Real4</td>
<td>0: 400.0</td>
<td>wavelength (lambda)</td>
</tr>
<tr>
<td>12</td>
<td>tg_mlam</td>
<td>angstrom</td>
<td>Real4</td>
<td>-400.00:400.00</td>
<td>Order times wavelength (m*lambda)</td>
</tr>
<tr>
<td>13</td>
<td>tg_srcid</td>
<td>Int2</td>
<td></td>
<td>0:32767</td>
<td>source ID, index from detect table</td>
</tr>
<tr>
<td>14</td>
<td>tg_part</td>
<td>Int2</td>
<td></td>
<td>0:99</td>
<td>HEG, MEG, LEG, HESF regions</td>
</tr>
<tr>
<td>15</td>
<td>tg-smap</td>
<td>Int2</td>
<td></td>
<td>0:32767</td>
<td>source map; flags for up to 10 sources</td>
</tr>
<tr>
<td>16</td>
<td>status[4]</td>
<td>Bit(4)</td>
<td></td>
<td></td>
<td>event status bits</td>
</tr>
</tbody>
</table>
Background Regions

The background is extracted in two regions: above and below the grating arm (background_up) and (background_down). The default spectrum widths are given in the tgextract help file.

There are two backgrounds because the geometry is not necessarily symmetric, especially for HETGS near the zero-order, or if there are other sources in the field. By default in Sherpa they are averaged.

Each PHA2 file has three keywords BACKSCAL, BACKSCUP, BACKSCDN, which scale the background counts arrays to represent the expected background counts in each of the source, BACKGROUND_UP, and BACKGROUND_DOWN regions.

For bright sources on ACIS-S, the background is likely negligible. However, in the HRC-S it is usually large.
Faint Spectra

Most X-ray objects are not as bright as Capella or NGC6624. In these cases, you might wish to co-add the grating data to increase the number of counts per bin. There are four possibilities:

1. **Co-add plus/minus orders of the same grating.** *Can broaden lines if zero-order is offset.*

2. **Co-adding HEG and MEG data.** *Complicates line shape function.*

3. **Co-adding separate observations.** *Instrumental background can vary, plus same issues of zero-order offsets.*

4. **Co-adding separate observations and instruments.** *All of the above.*
These calibration issues are either not a problem or are an “acceptable risk.” In this case, CIAO provides a number of tools:

**Adding together plus, minus orders**
```
add_grating_orders pha2=acisf00459N002_pha2.fits
   order=1 garm=MEG garf=acisf00459MEG_-1_garf.fits
```
```
garf=acisf00459MEG_1_garf.fits gtype=BIN gspec=10 root=459
```

**Adding together plus, minus orders**
```
add_grating_spectra pha1=2463_MEG_1_BIN10.pha
   pha2=459_MEG_1_BIN10.pha garf1=2463_MEG_1.arf
```
```
garf2=459_MEG_1.arf gtype=BIN gspec=10 root=3C273_summed
```
X Per, an HMXB observed for 50 ksec with the HRC/LETG.

```
add_grating_orders pha2=hrc_pha2.fits order=1 garm=LEG \
garf=x_perLEG_-1_garf.fits garfp=x_perLEG_1garf.fits \
gtype=BIN gspecl=1- root=xper
```

Co-add and bin this data with `add_grating_orders` to increase the number of counts/bin.
With low or moderate resolution data, one forward-folds models and compares to the data. With grating data, one can also measure line fluxes or equivalent widths directly.

However, many standard X-ray models are available only in Sherpa, XSPEC, or ISIS and so using these programs for grating analysis is common. All that is needed is the spectral data (pha2) file and the grating arf (and possibly rmf) files:
A sample sherpa session:

unix% sherpa
sherpa> data acis_pha2.fits
sherpa> paramprompt off
sherpa> rsp[hm1]
sherpa> rsp[hp1]
sherpa> rsp[mm1]
sherpa> rsp[mp1]
sherpa> hm1.rmf = acisheg1D1999-07-22rmfN0004.fits
sherpa> hm1.arf = acisf01318HEG_-1_garf.fits
sherpa> hp1.rmf = acisheg1D1999-03-22rmfN0004.fits
sherpa> hp1.arf = acisf01318HEG_1_garf.fits
sherpa> mm1.rmf = acismeg1D1999-07-22rmfN0004.fits
sherpa> mm1.arf = acisf01318MEG_-1_garf.fits
sherpa> mp1.rmf = acismeg1D1999-07-22rmfN0004.fits
sherpa> mp1.arf = acisf01318MEG_1_garf.fits
sherpa> instrument 3 = hm1
sherpa> instrument 4 = hp1
sherpa> instrument 9 = mm1
sherpa> instrument 10= mp1
sherpa> ignore allsets all
sherpa> notice allsets wave 14.9:15.4
sherpa> l1.pos = 15.014
sherpa> l2.pos = 15.079
sherpa> l3.pos = 15.2610
sherpa> freeze l1.pos
sherpa> freeze l2.pos
sherpa> freeze l3.pos
sherpa> fit
sherpa> lp 4 fit 3 fit 4 fit 9 fit 10
sherpa> import ("guide")
sherpa> mdl2latex
\begin{tabular}{lllllll}ModelName & Line Model & Position & Flux & Flux Error & Fit Data & Label \\
 & & Angstrom & ph/cm$^2$/s & ph/cm$^2$/s & \\l1 & delta1d & 15.014 & 0.00308923 & 6.7101e-05 & 3,4,9,10 & \\l2 & delta1d & 15.079 & 0.000270431 & 2.81612e-05 & 3,4,9,10 & \\l3 & delta1d & 15.261 & 0.00125857 & 4.79625e-05 & 3,4,9,10 & \\end{tabular}
And the results are shown here. \texttt{lp 4 fit 3 fit 4 fit 9 fit 10 gives}

![Graphs showing spectral analysis results](image)

while the \texttt{mdl2latex} command gives the table:

<table>
<thead>
<tr>
<th>ModelName</th>
<th>Line Model</th>
<th>Position</th>
<th>Flux</th>
<th>Flux Error</th>
<th>Fit Data</th>
<th>Label</th>
</tr>
</thead>
<tbody>
<tr>
<td>l1</td>
<td>delta1d</td>
<td>15.014</td>
<td>0.00308923</td>
<td>6.7101e-05</td>
<td>3,4,9,10</td>
<td></td>
</tr>
<tr>
<td>l2</td>
<td>delta1d</td>
<td>15.079</td>
<td>0.000270431</td>
<td>2.81612e-05</td>
<td>3,4,9,10</td>
<td></td>
</tr>
<tr>
<td>l3</td>
<td>delta1d</td>
<td>15.261</td>
<td>0.00125857</td>
<td>4.79625e-05</td>
<td>3,4,9,10</td>
<td></td>
</tr>
</tbody>
</table>
Alternatively (or in conjunction), ISIS, developed by the MIT CXC team, can be used in Sherpa or stand-alone.

```
unix% sherpa
sherpa> import("isis");
sherpa> load_data("acis_pha2.fits");
sherpa> plasma(aped);
sherpa> load_arf("acisf01318MEG_-1_garf.fits")
sherpa> assign_arf(1,9);
sherpa> flux_corr(9,2);
sherpa> d = get_data_counts(9);
sherpa> load_model("model.dat");
sherpa> fl = model_spectrum(d.bin_lo, d.bin_hi);
sherpa> g = brightest(10, where(ws(10,12)));
sherpa> id = open_plot("isis_capella.ps/vcps");
sherpa> resize(15);
sherpa> xrange(10,12);
sherpa> plot_data_counts(9);
sherpa> plot_group(g);
sherpa> close_plot(id);
```
**S-lang, Sherpa, and ISIS: Easy user-defined models**

Using *S-lang*, we can create a new power-law model quite easily:

```text
define slang_pow() {
    variable p, norm, Emin, Emax, dE, Result;
    if (_NARGS == 3) (p, norm, Emin) = ()
    if (_NARGS == 4) {
        (p, norm, Emin, Emax) = ()
        dE = Emax - Emin;
    }
    if (_NARGS == 3) Result = norm*(E^(-p));
    if (_NARGS == 4) Result = norm*(E^(-p))*dE;
    Result = typecast(Result, _typeof(Emin));
}
() = sherpa_register_model("slang_pow", ["power","norm"], 1, [1.0,1.e-2], % default values
                    [-10,1.e-20], % Minimum values
                    [10,1.e5], % Maximum values
                    [1,1]); % Both thawed by default
```
GUIDE is a collection of S-lang scripts whose purpose is to simplify access to the atomic database ATOMDB, which consists of the Astrophysical Plasma Emission Code (APEC) spectral calculations and the Astrophysical Plasma Emission Database (APED). GUIDE provides informational functions:

- **identify** Print finding chart of wavelengths
- **strong** List strong lines at a given temperature
- **describe** Describe atomic parameters of a line
- **mdl2latex** Convert fit parameters into a latex table
- **ionbal** Output ionization balance values for a given ion

These routines can be found in the directory `$ASCDS_BIN/interpreted`.

GUIDE can be run in either Sherpa or Chips, and is initialized in either case with the command

```plaintext
import(“guide”) 
```
The GUIDE command `identify` outputs line lists over a user-specified spectral range, along with an expected emissivity for each:

<table>
<thead>
<tr>
<th>$\lambda$(Å)</th>
<th>Ion</th>
<th>Upper</th>
<th>Lower</th>
<th>Emissivity</th>
<th>kT</th>
<th>RelInt</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.4403</td>
<td>Fe XX</td>
<td>158</td>
<td>9</td>
<td>2.23e-18</td>
<td>0.862</td>
<td>0.005</td>
</tr>
<tr>
<td>13.4440</td>
<td>Fe XX</td>
<td>116</td>
<td>8</td>
<td>8.75e-18</td>
<td>0.862</td>
<td>0.022</td>
</tr>
<tr>
<td>13.4440</td>
<td>Fe XXII</td>
<td>17</td>
<td>8</td>
<td>2.24e-17</td>
<td>1.085</td>
<td>0.055</td>
</tr>
<tr>
<td>13.4473</td>
<td>Ne IX</td>
<td>7</td>
<td>1</td>
<td>4.06e-16</td>
<td>0.343</td>
<td>1.000</td>
</tr>
<tr>
<td>13.4510</td>
<td>Fe XVIII</td>
<td>67</td>
<td>1</td>
<td>1.23e-17</td>
<td>0.685</td>
<td>0.030</td>
</tr>
<tr>
<td>13.4550</td>
<td>Ne IX</td>
<td>10205</td>
<td>19</td>
<td>1.74e-18</td>
<td>0.273</td>
<td>0.004</td>
</tr>
<tr>
<td>13.4550</td>
<td>Ne IX</td>
<td>10206</td>
<td>20</td>
<td>3.12e-18</td>
<td>0.273</td>
<td>0.008</td>
</tr>
</tbody>
</table>
More information on any given transition is available with the `describe` command:

**Ion Ne IX, energy level 1 –**
- electron configuration : $1s^2 1S_0$
- energy above ground (eV) : 0.000000
- Quantum state : $n=1$, $l=N/A$, $s=0$, degeneracy=1
- Energy level data source : 1983ADNDT..29..467S
- Photoionization data source : 1986ADNDT..34..415C

**Ion Ne IX, energy level 7 –**
- electron configuration : $1s^2p^1P_1$
- energy above ground (eV) : 922.609985
- Quantum state : $n=2$, $l=1$, $s=0$, degeneracy=3
- Energy level data source : 1983ADNDT..29..467S
- Photoionization data source : 1986ADNDT..34..415C

**Ion Ne IX, 1 – 7 interactions –**
- Electron collision rate from 1 $\rightarrow$ 7 : nonzero
- Reference bibcode : 1983ADNDT..29..467S
- Wavelength (lab/observed) (Angstrom): $13.447307 \pm 0.004000$
- Wavelength (theory) (Angstrom) : 13.470000
- Transition rate/Einstein A (s$^{-1}$) : $8.866670e+12$
- Wavelength (lab/observed) reference : 1988CaJPh..6..586D
- Wavelength (theory) reference : 1983ADNDT..29..467S
Given a “base” temperature, what lines should be so strong?
sherpa> strong(1.e7,5.e-17,5,25)

<table>
<thead>
<tr>
<th>Lambda</th>
<th>Ion</th>
<th>UL - LL</th>
<th>Emissivity@kT</th>
<th>RelInt</th>
<th>For More Info</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.1804</td>
<td>Si XIV</td>
<td>4- 1</td>
<td>5.14e-17 @ 0.862 0.103</td>
<td>describe(14,14,4,1)</td>
<td></td>
</tr>
<tr>
<td>6.6479</td>
<td>Si XIII</td>
<td>7- 1</td>
<td>8.77e-17 @ 0.862 0.175</td>
<td>describe(14,13,7,1)</td>
<td></td>
</tr>
<tr>
<td>8.4192</td>
<td>Mg XII</td>
<td>4- 1</td>
<td>6.89e-17 @ 0.862 0.138</td>
<td>describe(12,12,4,1)</td>
<td></td>
</tr>
<tr>
<td>9.4797</td>
<td>Fe XXI</td>
<td>248- 1</td>
<td>5.47e-17 @ 0.862 0.109</td>
<td>describe(26,21,248,1)</td>
<td></td>
</tr>
<tr>
<td>11.7360</td>
<td>Fe XXIII</td>
<td>20- 5</td>
<td>8.39e-17 @ 0.862 0.168</td>
<td>describe(26,23,20,5)</td>
<td></td>
</tr>
<tr>
<td>11.7700</td>
<td>Fe XXII</td>
<td>21- 1</td>
<td>1.94e-16 @ 0.862 0.388</td>
<td>describe(26,22,21,1)</td>
<td></td>
</tr>
<tr>
<td>12.1321</td>
<td>Ne X</td>
<td>4- 1</td>
<td>9.02e-17 @ 0.862 0.180</td>
<td>describe(10,10,4,1)</td>
<td></td>
</tr>
<tr>
<td>12.2840</td>
<td>Fe XXI</td>
<td>40- 1</td>
<td>5.01e-16 @ 0.862 1.000</td>
<td>describe(26,21,40,1)</td>
<td></td>
</tr>
<tr>
<td>12.3930</td>
<td>Fe XXI</td>
<td>40- 2</td>
<td>9.01e-17 @ 0.862 0.180</td>
<td>describe(26,21,40,2)</td>
<td></td>
</tr>
<tr>
<td>12.7540</td>
<td>Fe XXII</td>
<td>23- 6</td>
<td>7.17e-17 @ 0.862 0.143</td>
<td>describe(26,22,23,6)</td>
<td></td>
</tr>
<tr>
<td>12.8220</td>
<td>Fe XXI</td>
<td>83- 7</td>
<td>6.62e-17 @ 0.862 0.132</td>
<td>describe(26,21,83,7)</td>
<td></td>
</tr>
<tr>
<td>12.8240</td>
<td>Fe XX</td>
<td>60- 1</td>
<td>1.16e-16 @ 0.862 0.231</td>
<td>describe(26,20,60,1)</td>
<td></td>
</tr>
<tr>
<td>12.8460</td>
<td>Fe XX</td>
<td>58- 1</td>
<td>2.83e-16 @ 0.862 0.565</td>
<td>describe(26,20,58,1)</td>
<td></td>
</tr>
<tr>
<td>12.8640</td>
<td>Fe XX</td>
<td>56- 1</td>
<td>2.36e-16 @ 0.862 0.471</td>
<td>describe(26,20,56,1)</td>
<td></td>
</tr>
<tr>
<td>12.9120</td>
<td>Fe XX</td>
<td>51- 1</td>
<td>7.35e-17 @ 0.862 0.147</td>
<td>describe(26,20,51,1)</td>
<td></td>
</tr>
<tr>
<td>12.9650</td>
<td>Fe XX</td>
<td>48- 1</td>
<td>8.77e-17 @ 0.862 0.175</td>
<td>describe(26,20,48,1)</td>
<td></td>
</tr>
</tbody>
</table>
## Approximate

<table>
<thead>
<tr>
<th>Lambda</th>
<th>Ion</th>
<th>UL - LL</th>
<th>Emissivity@</th>
<th>kT</th>
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<td>13.0610</td>
<td>Fe XX</td>
<td>42–1</td>
<td>6.90e-17 @ 0.862 0.138</td>
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<td>13.3850</td>
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<td>71–1</td>
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<td>1.76e-16 @ 0.862 0.352</td>
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<td>14.2080</td>
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<td>55–1</td>
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<td>14.3730</td>
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</table>
The GUIDE *S-lang* functions can also be accessed via WebGUIDE:

http://obsvis.harvard.edu/WebGUIDE

More information on ATOMDB can be found at:

http://cxc.harvard.edu/atomdb

And, general questions about atomic rate calculations or line identifications can be posted on the new web forum AstroAtom:

http://cfa-www.harvard.edu/astroatom
Reprocessing grating data is recommended for optimal quality control; however, pha2 files from the archive are usually reasonable for assessing the data analysis needs.

Co-adding and/or binning grating data should be avoided when possible. Remember that, statistically, nothing is gained by it, although it may be much faster to fit it and easier to see the results.

Background subtraction and/or modeling are handled by Sherpa in a reasonable fashion, but more complex, wavelength-dependent subtraction could be done as well. User experimentation is recommended if the data warrant it.

A number of new facilities for atomic data analysis have been created, but the models still have limitations which should be kept in mind.