Spurion Quick Start

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Contents

List of Figures

1 Introduction

Just enough information to be dangerous. Please use the extensive on-line help in the program for detailed descriptions.

Spurion runs on jazz or any of the linux data collection computers. It can be used to make a plot of the scattering plane, accessible reciprocal space, and aluminum diffraction lines. Crystallography information can also be included as an option to color code the intensities of the Bragg peaks and systematic absences. Then the program can trace the wave vectors and energies for various higher-order scattering processes. Extensive help is available in the program itself, or on the web.

To run the program, type spurion at the prompt. The program opens two plot windows (reciprocal space, see Fig. 1, and an energy plot, see Fig. 2). The program itself is controlled from the main window by inputting commands at the prompt. (A GUI interface is planned for the future, but is not available presently).

Back to Section 1

2 Subsection of commands

dm: Start over with defaults or new files

The easiest way to get started is input a data file that has been collected and contains the information about the instrumental configuration and lattice. To do this use the command "**dm**" to load experimental parameters from an ICP data file. For example, if the filename is ybcom015.bt2, input "**2**", then "**ybcom015**", and then type "**d**" to get the crystallography defaults (Bragg peaks all have unit intensity; note that the lazy-pulverix info is used to calculate structure factors and systematic absences and is not necessary for spurion calculations).

a : Toggle plot aluminum Ewald spheres

To add aluminum lines to the reciprocal space plot, use the "**a**" command. Use it again to toggle the aluminum lines off.

s : Toggle plot higher-order scattering spurions

Use the "**s**" command to toggle the higher-order processes on and off. The trajectory of the second, third, and fourth order processes are shown on the reciprocal space plot, and the corresponding energy ranges are shown on the other plot.

i : Toggle plot incoherent scattering spurion

Use the "**i**" command to toggle the incoherent scattering process.

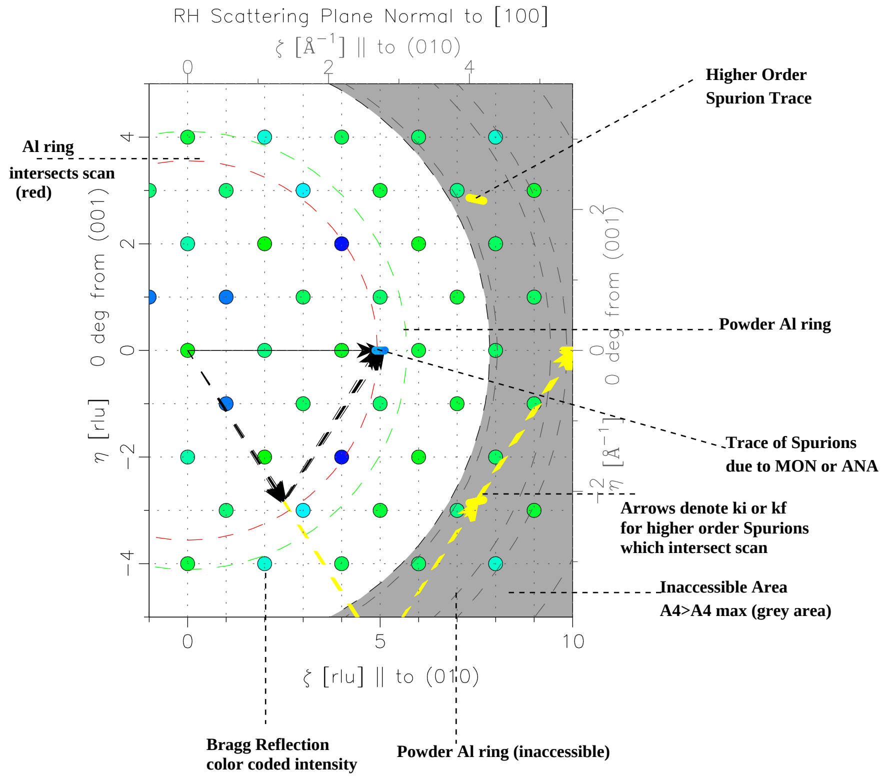

Figure 1: Spurion k-space diagram. Shows reciprocal space, showing the Bragg peaks, aluminum (sample holder) powder peaks (green if innocent, red if intersects the scan), and a few possible spurious processes (higher-order incoherent scattering shown with yellow arrows, red for elastic spurions).

Back to Section 1

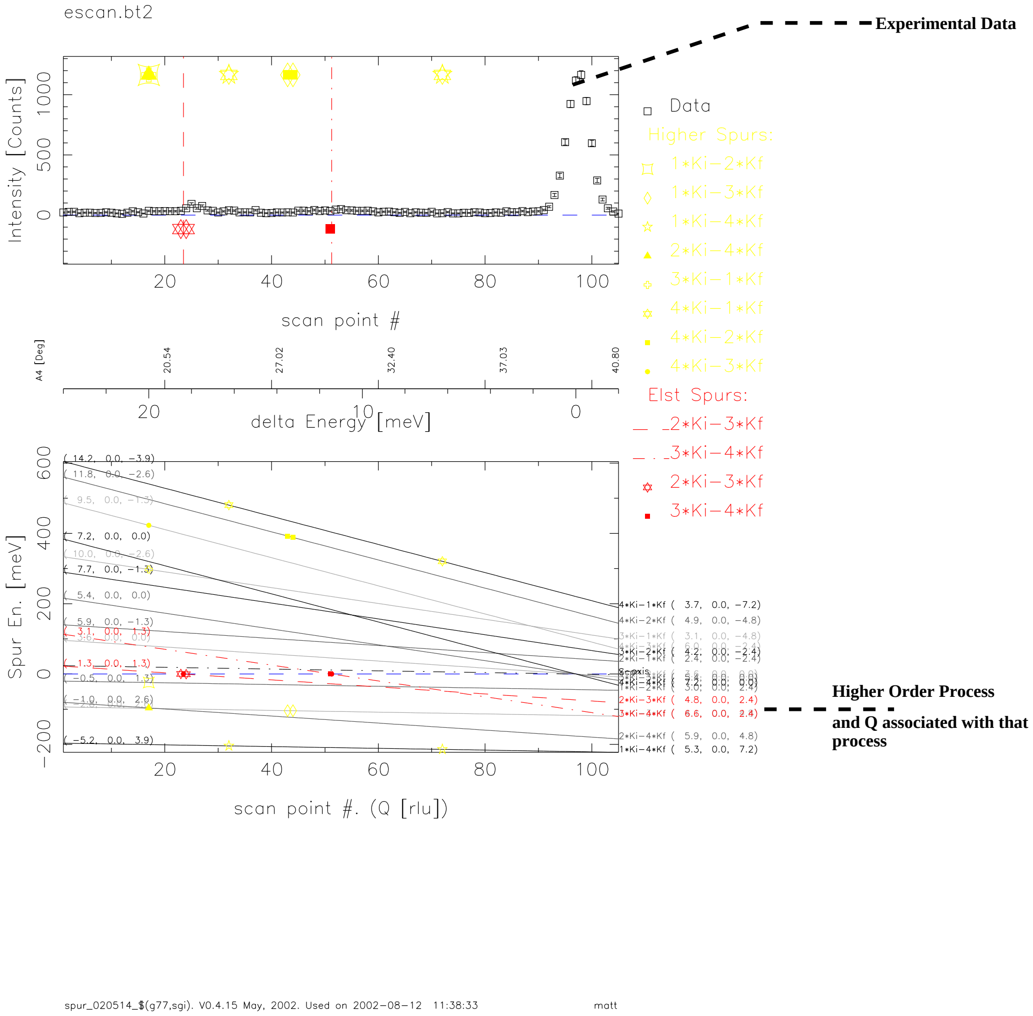

Figure 2: Spurion E-space diagram. Possible spurious elastic scattering is marked by the red dashed lines and the red symbols and labels. Possible higher-order processes are marked in yellow.

Back to Section 1

r : Rescale plot (reverse xmin and xmax for left)

Use the "**r**" command to rescale the reciprocal space plot.

z : Zoom spurion energy plot (0,0,0,0 for auto)

Use the "**z**" to rescale the energy plot.

pw: Printout/change graphics device

To get a hard copy, use "**pw**", then choose "**3**" to output a file ybcom015_cl.ps for a color postscript file of the reciprocal space plot that can be sent (outside of spurion) to the printer.

Back to Section 1

3 Background

A neutron incident on a sample with wave vector $\mathbf{k}_i$ and energy E_i is scattered into a final wave vector $\mathbf{k}_f$ and final energy E_f. The total momentum and energy must be conserved in the scattering process, and thus there must be a corresponding change in the crystal momentum and energy. The changes in wave vector Q and energy ΔE can be written as

$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f \tag{1}$$

and

$$\Delta E = \frac{\hbar^2 k_i^2}{2m_n} - \frac{\hbar^2 k_f^2}{2m_n} \tag{2}$$

The monochromator can scatter higher-order wavelength neutrons, and the analyzer can also scatter higher-order wavelength neutrons. So Eq. 1 can be written more generally as

$$\mathbf{Q}_{n,m} = n\mathbf{k}_i - m\mathbf{k}_f, \tag{3}$$

$$\Delta E_{n,m} = \frac{\hbar^2 n^2 k_i^2}{2m_n} - \frac{\hbar^2 m^2 k_f^2}{2m_n}. \tag{4}$$

Then when you perform a scan using Eqs. 1 and 2 with n=m=1 you are simultaneously scanning (inadvertently) using higher-order processes. We can use filters or monochromators/analyzers (such as silicon or germanium) that have systematic absences to eliminate some of these possibilities, but there are usually some processes that are possible. Spurion will show you where these processes occur in reciprocal space, and in energy.

Another possible spurious process can occur via incoherent scattering from the monochromator or analyzer crystal (or holder). If we have an incident wave vector $\mathbf{k}_i$, then a wave vector of the same length can scattering from the analyzer (i.e. $|k_i| = |k_f|$) via incoherent scattering. Conversely, you can scatter incoherently from the monochromator and then Bragg scattering from the analyzer. This is elastic scattering, and if the difference is close to a reciprocal lattice vector this process can produce a spurious peak, even though the incoherent cross section is orders-of-magnitude smaller than the Bragg scattering. The spurion program warns when this happens by color coding this elastic Bragg condition red.

Back to Section 1