Data Analysis and Visualization Tools for Resonant Inelastic X-Ray Scattering

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Background:

RXES is a process by which an incoming photon excites an electron in a core shell to the valence level. When the electron falls back to the core shell a photon is emitted with a different energy and momentum.

In this particular case we used RXES to observe the the change in oxidation states of the Europium under pressure. Europium can be in either +2 or +3 state at ambient temperatures and pressures but undergoes a shift under high pressures and becomes more dominantly trivalent. The energy of the scattered photon is different for each oxidation state. Through the use of RXES we can observe this change.

These particular measurements involve three different variables; Independent: incident photon energy, and detector angle; Dependent: photon count. By observing at which angles the photon count is maximized the energy of the scattered photons can be derived.

In this particular instance we are interested in deriving the ratio of the intermediate valence states of europium.

Methods:

This program is designed to find the ratio of the two seperate oxidations states. This is achieved through an optimized fitting algorithm. The data is broken up along the axis of the scattering angle to give a partial fluorescence yield (PFY) X-ray absorption spectra (XAS). Now the data is reduced to two dimensions. The data is now fit to a gaussian mixture model using *scipy.optimize.curve_fit()***.**

$$A_1 e^{(-(x-\mu_1 1)^2/(2*\sigma_1^2))}$$

$$+ A_2 e^{(-(x-\mu_2 1)^2/(2*\sigma_2^2))}$$

Where (A1, **μ**1, **σ**1, A2, **μ**2, **σ**2) are the varied parameters the functions is optimized for.

Each gaussian is then integrated individually. This is process is repeated for each detector angle until the entire data set has been fitted and integrated. The areas underneath both peaks are then respectively summed. The ratio of the areas beneath each peak is proportional to the ratio of atoms in each oxidation state.

Using the Pandas and Matplotlib Python libraries the data and results can be displayed in a number of ways including: a two dimensional density plot, a three dimensional surface plot, and if pressure is introduced as fourth variable, an animation of the change in the three dimensional surface plot.

Citations:

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