Step-Size Algorithm for Bonse-Hart Ultra-Small-Angle Scattering Instruments

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In USAS experiments, it is desired to step-scan the angle of the analyzer crystals, θ, in one scan through the entire angular range of interest, starting at an initial position of θ_{start} and taking N positions ending with θ_{end}. In this case, the step size would be:

$$\Delta\theta = \frac{\theta_{\text{end}} - \theta_{\text{start}}}{N-1}. \tag{1}$$

Unless the angular range is quite small, it is likely that the $\Delta\theta$ of Eq. 1 will be larger than the angular width of the Bragg reflection optics and the scan using this step size will fail to sample the intensity about the angular center, θ_c, of the rocking curve. Alternatively, it can be inconvenient to span the entire angular range with a constant step size $\Delta\theta = \Delta\theta_{\text{min}}$ where $\Delta\theta_{\text{min}}$ is the smallest step size to use while crossing the rocking curve peak of the Bragg reflection optics. Often, experimenters will thus divide the angular range into smaller intervals with different constant step sizes for each interval.

Ideally, a scan will employ a continuously-varying step size that will take constant-size small steps across the central part of the Bragg reflection and approximately proportionately larger steps as the angular distance from the Bragg reflection increases. One description of such an equation for the step size algorithm is that used in the UNICAT USAXS instrument[1]:

$$\Delta\theta_{i+1} = \Delta\theta_{\text{min}} + k|\theta_i - \theta_c|^\eta \tag{2}$$

In practice, the minimum step size, $\Delta\theta_{\text{min}}$, is chosen based on the smallest step of the θ rotary stage. Also, $\theta_1 \equiv \theta_{\text{start}}$. For the case $\eta = 1$, equal-log-spaced Q steps are taken in the tails of the rocking curve while constant sized steps are taken in the vicinity of θ_c. As η increases, larger steps are taken in the tails of the rocking curve (thus more points are packed towards θ_c). Typically, $\eta \sim 1.2$ gives good results. The parameter k is adjusted minimizing the error, ε, in arriving at the final step, θ_N:

$$\varepsilon = \theta_{\text{end}} - \sum_{i=1}^{N-1} \Delta\theta_{\text{min}} + k|\theta_i - \theta_c|^\eta = \theta_{\text{end}} - \theta_N \tag{3}$$

so that $|\varepsilon| \le \Delta\theta_{\text{min}}/2$.

In summary, k is determined from the user-specified terms of θ_{start}, θ_c, θ_{end}, N, and η using Eq. 3. Then, steps are generated as needed according to Eq. 2.

[1] `http://www.uni.aps.anl.gov/usaxs`