Increasing data collection rates by 10x via monochromator fly-scanning at PIPOXS

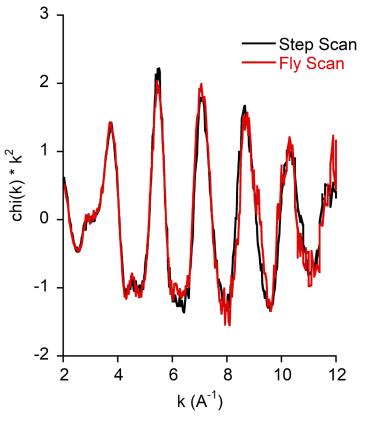
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What is the development?

Cornell University.

X-ray absorption spectroscopy (XAS) is a powerful technique for studying chemical catalysts that can provide information about an absorbing atom's geometry, oxidation state, and bond lengths. XAS experiments involve measuring how a sample absorbs x-rays across a range energies. During a typical experiment, a monochromator is used to select the energy of the x-rays being delivered to the sample, and this monochromator is then stepped through all desired energies one-by-one. Changing energy requires complex and precise synchronization of many independent mechanical motions. Traditionally, data is not collected while the motors are travelling between energies, which results in significant deadtime. Traditional step-scanning at the PIPOXS beamline is highly precise but limits how quickly an XAS scan may be collected, with the fastest possible scan being or order 10 minutes. This makes it impossible to perform time resolved XAS measurements on fast timescales.

To overcome these limitations, CHEXS has developed and implemented the ability to smoothly and synchronously scan all the monochromator motors through any energy range while data is continuously collected, eliminating discrete steps and their associated deadtime. Users can define an arbitrary number of regions to a scan with each region having a distinct energy increment size and count time. This flexibility allows XAS scans to be collected as quickly as the monochromator can move, allowing similar data quality to be obtained during an 80-second flyscan that previously required a 720-second stepped scan. Moreover, fly-scanning can be performed in both forward and reverse directions of the monochromator—data can be collected scanning to higher energy and also to lower energy—so that no time is lost at the end of a scan while the monochromator "resets" to the beginning.



An overlay of EXAFS data collected at the Pt L_3 -edge using a single 720 second stepped scan (black) and an 80 s fly-scan (red) that demonstrates the ability of fly-scanning to collect identical data quality in much faster times.



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What new experiments does this development enable?

Monochromator fly-scanning is applicable to both transmission and HERFD x-ray absorption experiments, which are core capabilities of the PIPOXS beamline, and which are both oversubscribed by users. Thus, the increase in throughput enabled by fly-scanning will have a profound impact on spectroscopy measurements conducted at CHEXS. Most directly, in favorable cases the time required per XAS scan has been reduced by nearly a factor of 10, allowing significantly more samples to be measured per day of beamtime, or equivalently, more user groups to be served per week of experiments. The ability to arbitrarily choose the exposure time per scan—down to under 60 s—will greatly reduce the need to attenuate the beam for radiation sensitive samples, allowing the high intensity incident x-rays to be fully utilized. Perhaps most importantly, monochromator fly-scanning will open up new time resolved experiments and enable chemical and structural changes to be probed on the seconds timescale, more an order of magnitude improvement over previous capabilities.

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