Energy-Position Dispersive X-ray Fluorescence

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The CSIRO Mineral Resources X-ray technologies group is at the forefront of developing industrial X-ray analysis instruments for the online measurement of elements, minerals, and shifts in chemical state. In this study, we present an innovative improvement to in-situ X-ray fluorescence (XRF) spectroscopy that provides high energy resolution.

Our novel method, called Energy-Position dispersive X-ray fluorescence (EPDXRF), is an extension of the state-of-the-art technique Position dispersive X-ray Fluorescence (PDXRF) [1], [2]. Unlike traditional XRF methods that scan through energy levels or have poor energy resolution, EPDXRF simultaneously disperses and measures a selected range of X-ray energies using a CCD detector, a Polycapillary optic, a flat lithium fluoride crystal cut on the 220 plane, and a low-power X-ray tube. The X-rays are focused onto the sample where XRF occurs, and then dispersed onto the flat lithium fluoride crystal, where they undergo Bragg diffraction depending on the angle of incidence and energy. The diffracted X-rays are then simultaneously detected by different strips of the CCD detector, allowing both the position and energy information of X-rays to be stored.

By dispersing the X-rays through Bragg diffraction, we achieve an unprecedented energy resolution of 3eV, making it possible to apply sophisticated background reduction techniques to the spectra. As demonstrated in Figure 1, a Monte Carlo simulation of the copper K-spectra shows a remarkable 50% reduction in background across the entirety of the spectra and an even more significant 90% reduction on the right of the Kβ peak. This reduction in background enables precise measurements of shifts in the chemical state of a material, which has significant implications for battery development and other redox reactions. Additionally, our technique allows for the measurement of low-intensity satellite structures in XRF spectra, providing valuable insights into the inner structure of atoms.

Figure 1. Monte Carlo simulation of the Copper Kα and Kβ spectra using both the PDXRF [2] and EPDXRF technique respectively. The background is reduced by approximately 50%.
