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Advanced Processing of High-Pressure Data from CCD Detector System. Michael Ruf, Bruker AXS Inc., 5465 East Cheryl Parkway, Madison, WI, USA.

A major challenge in the field of High Pressure crystallography is the acquisition of sufficient quality data for a successful structure determination especially for low symmetry samples. The volume of reciprocal space accessible for X-ray examination is constrained by the shape and size of the Diamond Anvil cell used and mostly determined by its opening angle. In addition the acquired data suffer from absorption effects from the Diamond Anvils, high background and Beryllium powder diffraction as well as overlapping of sample reflections with those from the diamonds used in the experiment.

The advantages of using CCD detectors in the field of high-pressure single-crystal structure determination have been well recognized in recent years. Modern 3- and 4-axes goniometers equipped with a CCD detector allow the acquisition of virtually all accessible data. These diffraction systems are very sensitive and fast with highly automated software for strategy planning, data acquisition and data processing.

This presentation will focus on recent advances in software development which help tackling the problems with data acquired in high-pressure experiments as outlined above. We will present new algorithms for data integration for simultaneous processing and deconvolution of reflections from the sample and the diamond reflections.