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Combined XRD and Raman Combinatorial Screening System. Bob He, Chris Frampton, Juergen Sawatzki, Bruker AXS, 5465 East Cheryl Parkway, Madison, WI 53711 USA.

Combinatorial investigations require rapid screening techniques to test and evaluate variations of composition, structure and property within a material library. X-ray diffraction provides abundant information on the atomic arrangement of the sample revealed through the diffraction pattern. Raman spectroscopy measures the characteristic vibration frequencies determined by the chemical composition and chemical bond. Both X-ray diffraction and Raman spectroscopy are non destructive methods that require virtually no sample preparation, thus, allowing samples to be analyzed simply and quickly in their natural form. Combinatorial screening based on spectroscopic and diffraction techniques is of high importance *e. g.* for drug substances and formulations since the polymorphism of active ingredients has to be controlled to achieve a reliable product quality which will satisfy the regulatory authorities.

This presentation covers the development of an innovative instrument consisting of XRD and Raman spectroscopy for combinatorial screening. The X-ray source, X-ray optics, X-ray detector, laser source, Raman probe and an auto-zoomed video microscope are all integrated into a single platform so that the X-ray diffraction pattern, Raman spectrum and optical image from the same sample or sample area can be measured in a single load. The software associated with the system can treat data from the various techniques and analyze the results in correlation.