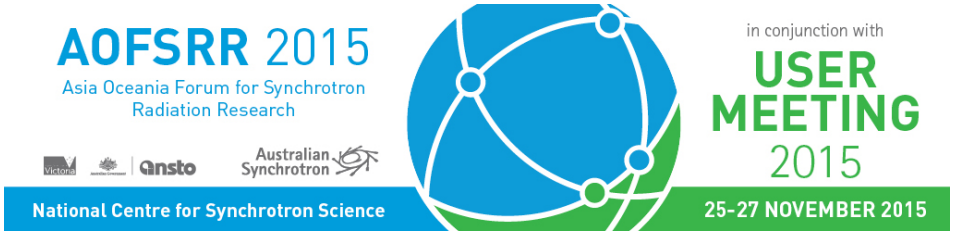

Contribution ID : **21** Type : **Oral**

Technique for the Identification of Phases and Phase Transformations in In Situ Diffraction Data

Friday, 27 November 2015 15:05 (20)

In situ X-ray diffraction is a common technique for observing and determining structural transitions in crystalline materials with changes in temperature, pH, pressure, or some other driving force. In the analysis of metal hydride systems, there can be structural transitions composed of multiple phases forming and decomposing simultaneously. These patterns are often overshadowed by high intensity peaks, leaving the subtle phase transitions undetected by conventional automated techniques. We are developing an automated method based on wavelet peak identification and diffraction pattern derivatives to separate and identify these subtle phase transitions. The method will include peak-to-phase assignment and possibly indexing.

Keywords

diffraction; peak identification; phase transformation; automation; in situ

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Session Classification : Techniques II

Track Classification : Beamlines, Instrumentation and Techniques