

Abstract Submitted
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Advanced Spectral Analysis Program (ASAP) for High-Pressure X-ray Diffraction JEFFREY MONTGOMERY, Lawrence Livermore Natl Lab — A program for analyzing large powder diffraction data sets has been developed. This tool enables the user to fit any type of crystal structure by indexing peaks in multiple files simultaneously by manually selecting them from a 2D plot of peak positions. The program has tools for automatic peak fitting and pressure determination using various equations of state. The interface is useful for correlating information from various types of spectral data, and so tools have been added for analyzing common fluorescence markers such as ruby, strontium tetraborate, and diamond. The program operation is demonstrated by the analysis of high-pressure powder x-ray diffraction data taken on a sample of vanadium metal at the Advanced Photon Source 16-BMD beamline. Samples were compressed in three runs to a pressure of 70 GPa in an attempt to measure the phase transition from bcc to orthorhombic in hydrostatic and non-hydrostatic conditions. Using ASAP to analyze this data provides a fast and accurate tool for observation of such a subtle transition, which is characterized primarily by a narrow splitting of the bcc 110 and 112 peaks. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

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