21-Crystallography at Non-Ambient Temperatures and/or Pressures: Phase Transitions

21.01 - High Pressure Crystallography

**REFERENCE**

**REFERENCE**
McMahon, M. I., McElhaney, R. J., and Neves, Department of Physics, The University of Edinburgh, U.K.

**REFERENCE**
Hamaya, N., Department of Physics, Ochanomizu University, Japan.

Recent developments of high-pressure diffraction experiments at the Photon Factory, KEK, will be briefly reviewed with special emphasis on accurate crystal structure determination, which is now feasible by using reliable intensity data collected with either a combination of the DAC and a imaging plate, or a large volume apparatus, MAX80, operated in an angle-dispersive mode. The former technique has been applied to the study of fcc-distorted fcc phase transition in Pr and La. With the aid of a Rietveld analysis, we have identified the crystal structure of the distorted fcc phase to be R 3 2/m (Dl), with Z = 8, determined its positional parameters as a function of pressure, and suggested the association of phonon softening with this transition. In the case of La, its novel re-entrant phase transition scheme, fcc-rhombohedral-fcc, is quantitatively followed in the variation of positional parameters with pressure. Angle-dispersive diffraction on MAX80 is currently carried out using monochromatic high-energy X-rays with E> 40 keV in order to avoid large absorption in the material surrounding the sample. High angular resolution D = 0.05° FWHM and high S/N ratio capability has enabled us to study a complex crystal structure of Bi and MnmF2 at high pressures and high temperatures.