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Diffraction Studies of Single Crystals at High Pressure using Synchrotron Radiation. Suhithi M. Peiris, NAVSEA, Indian Head, MD, PeirisSM@ih.navy.mil, Ray Butcher, Howard Univ., Washington, DC, Wayne Pearson, US Naval Academy, Annapolis, MD.

Most diffraction studies of single crystals at high pressure use in-lab radiation sources. [1] A few studies have used synchrotron radiation. [2] The restricted cone angles on a diamond anvil cell (DAC) severely limit the spots per pattern, especially when Be plates are not used.

We have done angle-dispersive x-ray diffraction experiments of single-crystals in DACs at high pressure at Cornell University's synchrotron source (CHESS). Our samples were small molecular crystals loaded in Merrill-Bassett type DACs without Be plates, mounted on a two-circle Diffractometer. The DAC was oscillated over 4° around an axis perpendicular to the x-ray beam. Data were obtained at 1, 2 and 3.5 GPa. An existing data analysis package (DPS/Mosflm/CCP4) was used for indexing and peak integration. Structure factors were obtained at 1 GPa and structural analysis was performed using MaXus. The 2 and 3.5 GPa data indicates a phase change or a twinned crystal.

Block et al., Science, 1965, 148, 947; Hazen et al., American Mineralogist, 1989, 74, 352; Dera, et al., Phys. Rev. B, 2002, 65, 134105.

Fourme et al., J. of Synch. Rad., 2001, 8, 1149; Allan et al., J. of Synch. Rad., 2001, 8,10; Hejny et al., Acta Cryst., 2002, A58 (Supplement), C175