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Dffraction Studies of the P-T Phase Diagram with Single-Crystal Ca122 A.I. GOLDMAN, A. KREYSSIG, Ames Laboratory/Department of Physics and Astronomy, K. PROKES, Helmholtz-Zentrum Berlin für Materialien und Energie, D.K. PRATT, Ames Laboratory/Department of Physics and Astronomy, D.N. ARGYRIOU, Helmholtz-Zentrum Berlin für Materialien und Energie, J.W. LYNN, NCNR, Gaithersburg, MD 20899, S. NANDI, Ames Laboratory/Department of Physics and Astronomy, S.A.J. KIMBER, Helmholtz-Zentrum Berlin für Materialien und Energie, Y. CHEN, NCNR, Gaithersburg, MD 20899, Y.B. LEE, G. SAMOLYUK, Ames Laboratory/Department of Physics and Astronomy, J.B. LEAO, S.J. POULTON, NCNR, Gaithersburg, MD 20899, S.L. BUDKO, N. NI, P.C. CANFIELD, B.N. HARMON, R.J. MCQUEENEY, Ames Laboratory/Department of Physics and Astronomy — Single crystal neutron and high-energy x-ray diffraction have identified the phase lines corresponding to transitions between the ambient-pressure tetragonal (T), the antiferromagnetic orthorhombic (O) and the nonmagnetic collapsed tetragonal (cT) phases of CaFe2As2. We find no evidence of additional structures for pressures up to 2.5 GPa (at 300 K). Both the T-cT and O-cT transitions exhibit significant hysteresis effects and we demonstrate that coexistence of the O and cT phases can occur if a non-hydrostatic component of pressure is present.

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