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High Pressure X-ray Diffraction Studies on ZrFe_2 : A Potential Hydrogen Absorption Medium

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BACKGROUND

The potential application of intermetallic compounds (IMC) under high hydrogen pressure in studies of hydrogen sorption properties is defined by two important properties. Intermetallics of Laves phases have a suitable binding energy for hydrogen which allows its absorption or desorption near room temperature and atmospheric pressure. High pressures allow to efficiently interact hydrogen with intermetallics, which were considered nonhydride forming [1,2]. For example, ZrFe_2 , ZrCo_2 , and ZrFe_2 possess fairly high hydrogen absorption capacity at high pressures [3]. A nonactivated ZrFe_2 sample starts to interact with hydrogen only at 80 MPa, while equilibrium absorption and desorption pressures of the activated alloy on a plateau are 69 and 32.5 MPa, respectively. Even though ZrFe_2 and related Laves phases are subjected only to moderate hydrogen pressures during absorption and desorption, it is essential to understand the structural phase stability under variable pressure-temperature conditions. The present investigation is aimed to study the pressure induced structural changes in ZrFe_2 using synchrotron powder x-ray diffraction. High pressure structural studies were performed up to 50 GPa using a diamond anvil cell in the angle dispersion geometry.

EXPERIMENTAL

High purity (99.9%) ZrFe_2 bulk powder obtained from sigma Aldrich was used for high pressure experiments. The powder was well ground in an agate mortar and pelletized. A small piece from the dense pellet was loaded with a few ruby grains in a Re gasket with a 150 μm hole of a symmetric type diamond anvil cell (culet 320 μm). 4:1 methanol ethanol mixture was used as a pressure medium. The pressure in the cell was measured with an offline ruby system. The data collection was performed at room temperature with incident synchrotron x-rays of wavelength 0.37571 \AA at ID-B station of HPCAT. A MAR 345 imaging plate was used to collect the diffraction images up to 50 GPa. The detector to sample distance was calibrated using a CeO_2 standard. The XRD images were then integrated using FIT2D. The structural analysis of the patterns was carried out using the JADE software package.

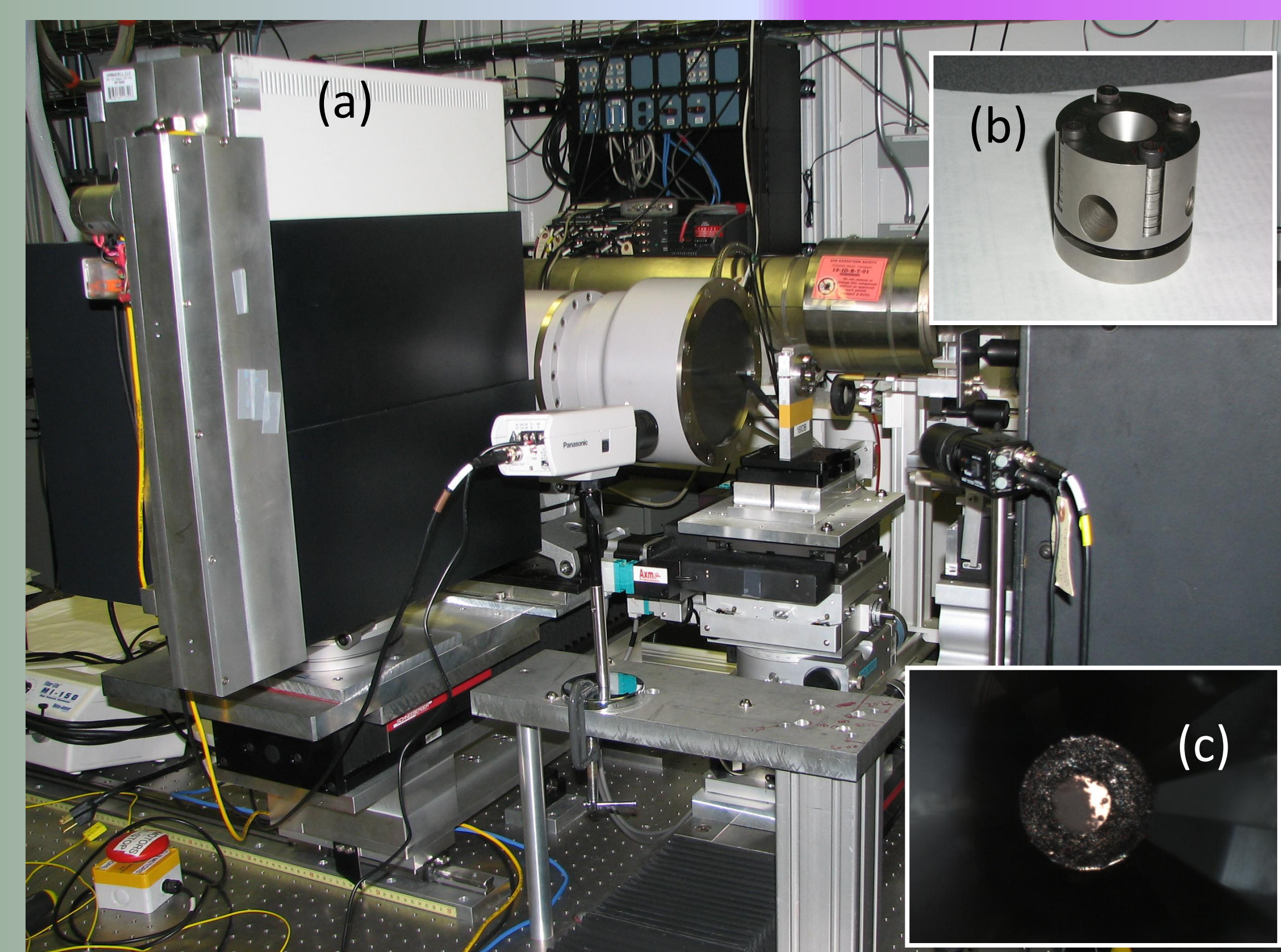
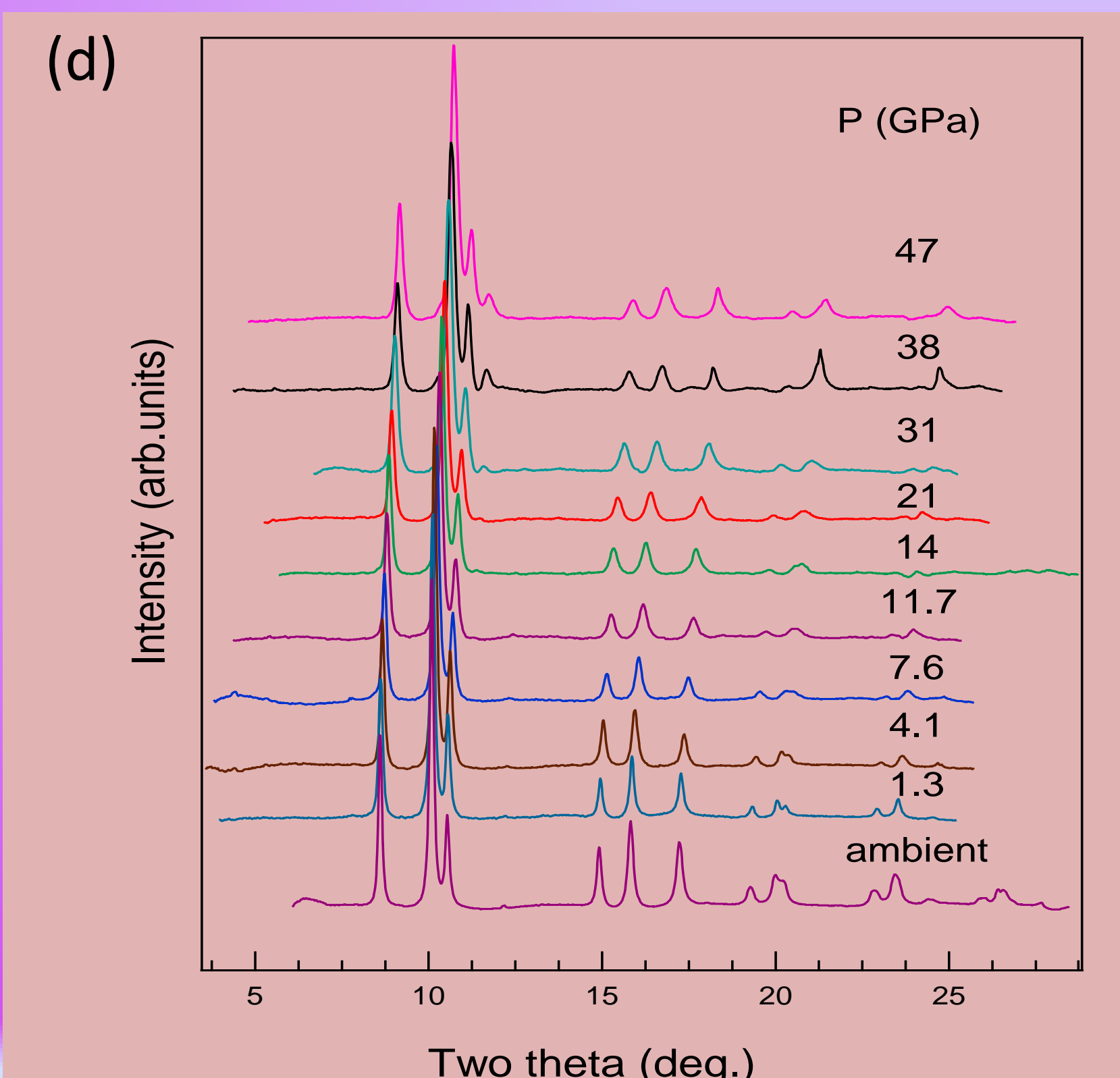


Fig.1 (a) High pressure x-ray diffraction set up at ID-B station at HPCAT, Argonne National Laboratory (b). Symmetric type high pressure diamond anvil cell. (c). ZrFe_2 sample in the gasket of DAC with ruby grains. (d). X-ray diffraction patterns collected at various pressures for ZrFe_2



RESULTS

The x-ray diffraction patterns collected at various pressures are shown in Fig.1 (d). Analysis of the x-ray diffraction images at nearly ambient pressure and temperature conditions showed Fd3m cubic structure. The experimental cell parameter obtained at ambient pressure $a=7.10026 \text{ \AA}$ compares well to the value reported in literature for this material 7.0757 \AA [4,5]. The d-spacings plotted as a function of pressure showed gradual decrease as pressure was increased (Fig.2 (a)). Up to 21 GPa, the diffraction patterns show no abrupt changes indicating no structural changes. Above 21 GPa, a new peak around 11 degrees started to appear. This new peak may indicate a possible structural change or distortion. Careful structural analysis is under progress to understand further details. The unit cell volume was obtained for each pressure and plotted as shown in Fig. 2(b).

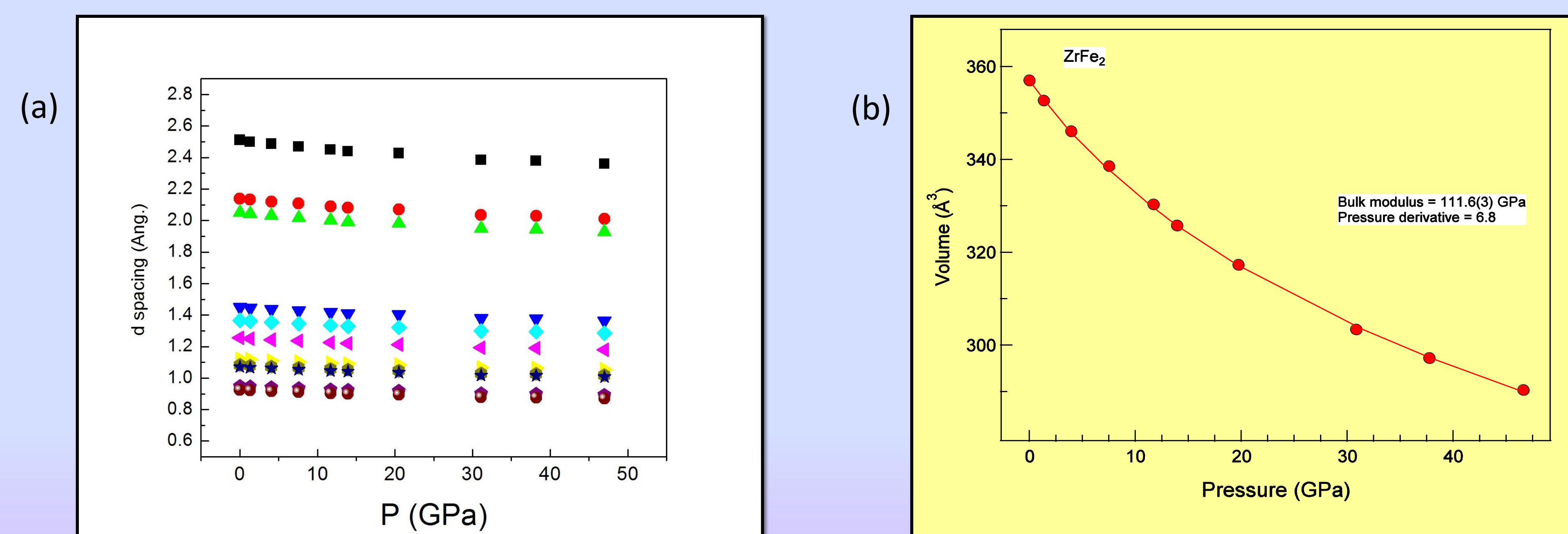


Fig.2 (a). Variation of d values of ZrFe_2 cubic Laves phase as a function of pressure (b). P-V plot of ZrFe_2

CONCLUSIONS AND SUMMARY

High pressure diffraction studies on ZrFe_2 sample were performed under varying pressures up to 50 GPa. The experiments showed a gradual decrease in cell parameter, volume, and d-spacing as pressure increased. No pressure induced transition is observed up to 21 GPa. Above 21 GPa we inferred a new diffraction peak emerging around 11° . Detailed structural analysis is under progress. The bulk modulus for the Fd3m cubic phase is obtained to be 111.6(3) GPa and it agrees well with the compressibility of similar AB_2 type intermetallic compounds [6].

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