Experimental Report

27/06/2014

Proposal: **5-31-2250** **Council:** 4/2012

Title: Pressure induced delocalization ina G-type antiferromagnet BaMn2As2

This proposal is a new proposal

Researh Area: Physics

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Samples: BaMn2As2

Instrument	Req. Days	All. Days	From	To
D20	3	3	09/11/2012	12/11/2012

Abstract:

Pressure induced metallization has been observed at ~4 GPa in G-type antiferromagnet BaMn2As2 using temperature dependent resistivity measurements. RT XRD measurements suggest that the metallization is not associated with a structural change. It is proposed to investigate evolution of the magnetic ground state across this insulator to metal transition using high pressure neutron diffraction. Temperature dependent high pressure neutron diffraction will be able to identify the origin of the transitions observed in high pressure resistivity data and clarify whether these anomalies arise from structural or magnetic origins.

"Pressure induced delocalization in a G-type antiferromagnet $BaMn_2As_2$"

$BaMn_2As_2$ is a G-type antiferromagnet (T_N =625K) with Mn moments aligned along c-axis and has insulating ground state [1]. Band structure calculations, resistivity and specific heat measurements [2] indicate that $BaMn_2As_2$ is semiconductor with a small band gap of 0.2 eV. Our recent high pressure measurements of resistivity and XRD have shown $BaMn_2As_2$ undergoes insulator to metal (IM) transition at around 5 GPa, which is also associated with an isostructural electronic transition [3]. Hence, it is of great interest to explore what happens to its magnetic structure when an external pressure is applied. With this aim in mind, neutron diffraction experiments at high pressures up

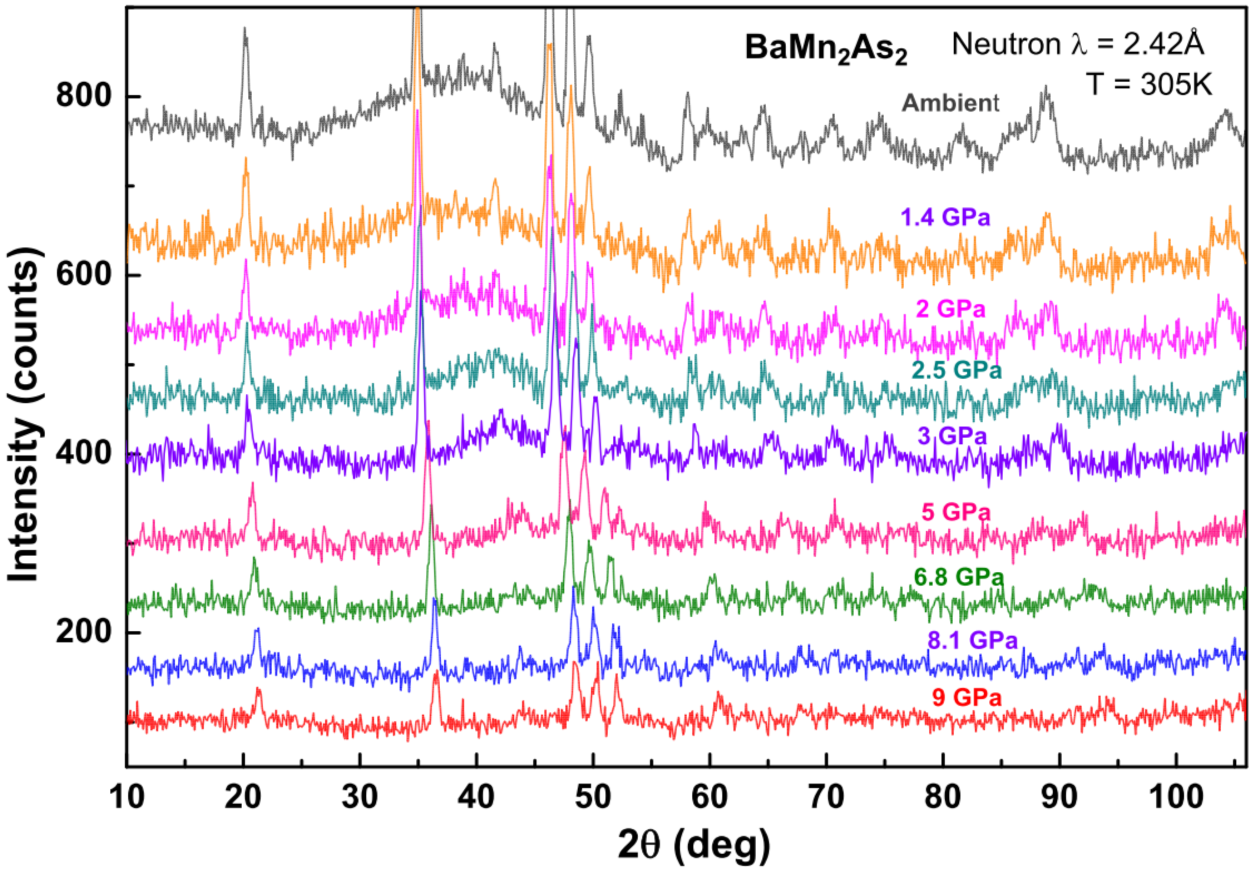

Figure 1. Neutron diffraction patterns recorded at T = 305K as function of temperature on $BaMn_2As_2$ compound using a wavelength of 2.42Å.

to 10 GPa as function of temperature were performed at Institut Laue Langevin (ILL) using D20 diffractometer. Temperature dependent neutron diffraction patterns were recorded from 80K to 9K at some selected pressures. Neutron diffraction data were also collected as function of pressure up to 9 GPa at room temperature as shown in figure 1. The structure at room temperature remains more or less same on application of high pressures up to 9 GPa. Shift in Bragg peaks to higher scattering angles indicating lattice contraction was observed. These experiments suggest that high pressures (up to 9 GPa) at room temperature does not affect the room temperature G-type AFM order that is present in this compound. Temperature dependent diffraction data taken at 3 GPa does not show any significant changes in the patterns down to 9K.

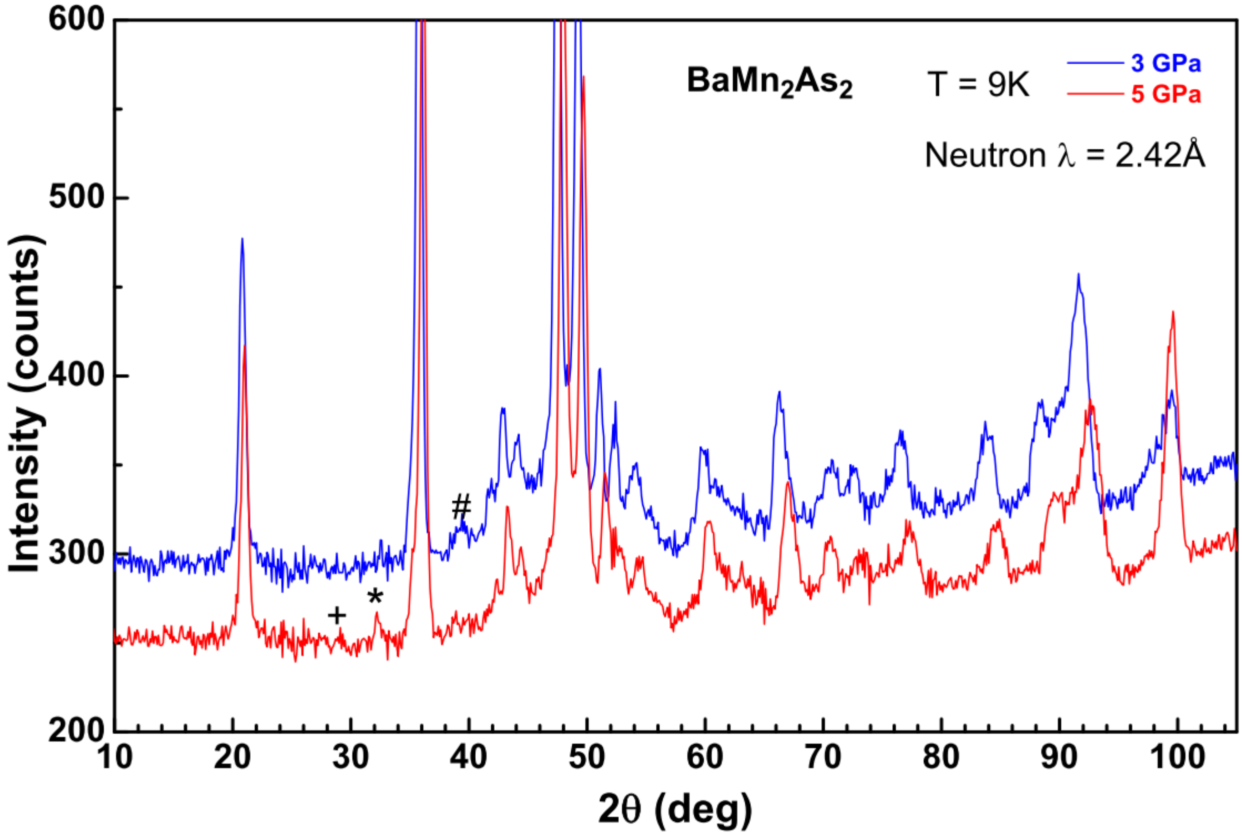

Figure 2. Neutron diffraction patterns at 9K cooled different pressures 3 GPa and 5 GPa. Symbols '*', '#' and '+' indicate the changes brought in by the application of pressure.

However, when the pressure is increased to 5 GPa, certain changes in the patterns are noticed at low temperatures as shown in figure 2. The peak (~32.16°) marked with asterisk (*) appears at 5 GPa while peak (~39.06°) marked as '#' disappears. There is also another very weak peak at 29.15° (marked as '+'). All these changes observed at 5 GPa are present only at low temperatures from 80K downwards and these are not present at room temperature. All the major magnetic peaks remain intact indicating that the G-type AFM order is still preserved but there may be minor modifications in magnetic structure and/or small structural distortions. Detailed analyses of all the neutron data are being carried out at present which are expected to through more clarity on these aspects.

[1] Yogesh Singh, *et al*. Phys. Rev. B **80**, 100403 (2009)
[2] Jimming An *et al*, Phys. Rev. B **79**, 075120 (2009)
[3] A.T. Satya, *et al*, Phys. Rev. B **84** 180515 (2011)