ESRF	**Experiment title:** Evolution from Itinerant Ferromagnet to Quantum Critical Line in the Weak Itinerant Ferromagnet $ZrZn_2$ – A High Pressure, Low Temperature Structural Study	**Experiment number**: HS4057
Beamline: ID09A	**Date of experiment**: from: 31/3/2010 to: 03/04/2010	**Date of report**: 28/02/2011
Shifts: 9	**Local contact(s)**: Dr. Michael Hanfland	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Proposer: Dr Emma Pugh*, Cavendish Laboratory, University of Cambridge, Cambridge, UK

In addition to the proposer the following attended and helped during the experiment:
Ms Lara Sibley* (PhD Student), Cavendish Laboratory, University of Cambridge, Cambridge, UK

Report:

We have measured the crystal structure of $ZrZn_2$ with increasing pressure from 0 to 20 GPa by performing powder diffraction measurements on beamline ID09A inside a diamond anvil cell both at room temperature and at 10 K. $ZrZn_2$ crystallises in the cubic C15 Laves phase structure at ambient pressure and temperature. At low temperature $ZrZn_2$ has ferromagnetic order with a Curie temperature of 28.5 K at ambient pressure. As pressure is applied to ferromagnetic $ZrZn_2$ the magnetic ordering temperature is suppressed to around 0.9 GPa at 10K (2 GPa at 50mK). The nature of the magnetic state and any new quantum states observed on the border of magnetism are closely related to the crystal structure and hence the motivation for this study. An as yet unidentified new quantum state has been observed in resistivity measurements in $ZrZn_2$ above the magnetic suppression pressure at low temperature ($T<15K$). Our measurements at the ESRF have allowed us to study the changes in crystal structure which occur in this region of the $ZrZn_2$ phase diagram.

In our ESRF measurements we have observed clear evidence for a volume instability in $ZrZn_2$ around 0.8-1.0 GPa as the pressure was increased at 10K. Figure 1 shows that there is a clear change in gradient of the lattice parameter compression in this region. This corresponds to the pressure at which the ferromagnetic ordering temperature is suppressed at 10K with the corresponding observation of unusual power laws in resistivity data which occur at the quantum phase transition. We have seen no evidence for a volume instability as the pressure was increased at room temperature when the sample was paramagnetic throughout the whole pressure range studied indicating the significance in the collapse of the ferromagnetic order to the volume instability.

We have performed structural refinement of the powder diffraction data using the GSAS software and have seen no evidence for a structural phase transition up to the highest pressure studied of 20 GPa (fig 2) either at low temperature or room temperature. This shows that there are subtle, but significant structural changes that are occurring at the quantum phase transition on the border of ferromagnetism and that these are likely to have a bearing on the magnetic order and nature of the new quantum state observed in our resistivity data. The low temperature data is being used to perform density functional theory and energy calculations on $ZrZn_2$.

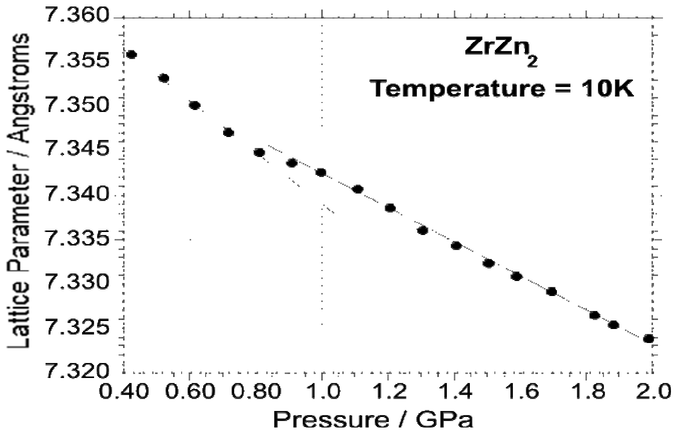

Figure 1 – Pressure dependence of the lattice parameters for $ZrZn_2$ at 10K obtained from high pressure, low temperature powder diffraction study at ESRF (ID09A). Between 0.8 and 1.0 GPa there is a clear discontinuity in the lattice parameter. This corresponds to the pressure at which the ferromagnetic ordering temperature is suppressed at 10K with the corresponding observation of unusual power laws in resistivity data. (Lines are guide to the eye).

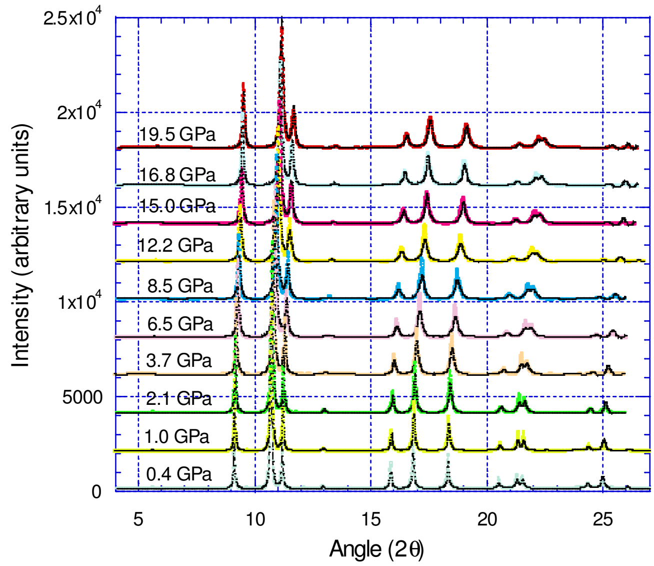

Figure 2 – Powder diffraction data of $ZrZn_2$ at 10 K at different pressures. For each pressure curve the coloured lines are from the experimental data and the black lines are the fitted refinement using the GSAS software package.