ESRF	**Experiment title:** How to extract the entropy from accurate P(V,T) measurements? Implication on the Alpha-Gamma phase transition in Cerium.	**Experiment number**: HS 2991
Beamline: ID09A	**Date of experiment**: from: 14 June 2006 to: 17 June 2006	**Date of report**: 28 August 2006
Shifts: 9	**Local contact(s)**: Michael Hanfland	*Received at ESRF:*

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Report:

One of the most promising theoretical techniques to study the α–γ phase transition of cerium is the LDA+DMFT scheme which is a combination of density functional theory (DFT) within the local density approximation (LDA) with dynamical mean-field theory (DMFT). Recently, cerium has been the focus of several theoretical works utilizing this framework. Among those, two of these studies are mainly aimed at calculating the internal energy U as a function of the cell volume, and a disagreement in the behavior of U(V) was seen between these two implementations of the LDA+DMFT scheme. In one case, U(V) features a region of negative curvature while in the other case the curvature is always positive. This raises the important question of the role of entropy in this transition.

To address this question, we were allocated 9 shifts of beamtime on ID09A in June 2006 to perform precise measurements of pressure versus volume curves across this phase transformation by varying the temperature by small steps in the 350 K range. With this respect, accurate free energy differentiates could have been computed, and both the entropy S and the internal energy U could have been evaluated with a good precision. Following our proposal, we brougth 3 diamond anvils cells (DAC) setup for low-pressure work and higly stable pressure settings, using neon as a pressure transmitting medium.

This was the first attempt ever to study Cerium while utilizing a hydrostatic pressure transmitting medium (neon) loaded using a high pressure gas vessel. Unfortunately, we have underestimated the high cerium reactivity with the atmosphere during our DAC loadings: while the sample handling and positioning into the DAC was performed in suitable conditions (glove-box filled with anhydrous argon), we wrongly assumed the tightened DAC was leak-proof enough to be carried from the glove box to the gas loading vessel without special precaution.

Since there was no way to check for the sample oxydation without x-rays, this has resulted in figuring out at the ESRF that all our three samples were oxydized and useless to carry out the project. The recorded diffraction patterns showed a CeO_2 presence while no metallic Ce peaks was to be seen.

We won't ask for more beamtime for this project in the next run: we first have to solve the issue of how to carry a diamond anvils cell containing a highly reactive sample from our glove box to our gas loading vessel. For this purpose, a container aimed at preserving the sample from the atmosphere and transfering it to the vessel is being developped and should be ready by the 1st semester of 2007.