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ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office using the **Electronic Report Submission Application:**

http://193.49.43.2:8080/smis/servlet/UserUtils?start

Reports supporting requests for additional beam time

Reports can now be submitted independently of new proposals – it is necessary simply to indicate the number of the report(s) supporting a new proposal on the proposal form.

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Deadlines for submission of Experimental Reports

- 1st March for experiments carried out up until June of the previous year;
- 1st September for experiments carried out up until January of the same year.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report, in English.
- include the reference number of the proposal to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** High pressure study of PbRuO$_3$	**Experiment number**: hs4175
Beamline: ID09	**Date of experiment**: from: 11/09/2010 to: 14/09/2010	**Date of report**: 28.2.2011
Shifts:	**Local contact(s)**: Michael Hanfland	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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Report:

Transition metal oxide perovskites display a remarkable range of electronic phenomena such as superconductivity, colossal magnetoresistances, and other properties resulting from coupled charge, orbital and spin orderings. PbRuO$_3$ is a high pressure perovskite with very differently physical properties to other ARuO$_3$ perovskites. [1] Previous synchrotron x-ray and neutron powder diffraction had show a remarkable first order symmetry reversing phase transition in PbRuO$_3$ at 75 K. This unusual subgroup (Pnma) to group (Imma) transition is coupled with an orbital ordering transition, creating planes of minority-spin occupied d$_{xy}$ orbitals at low temperatures. The orbital disorder provides a large positive entropy contribution to the phase transition on warming, outweighing the negative entropy of the symmetry-lowering structural contribution. No long range magnetic order is evident down to 1.5 K.

Both high and low temperature phases of PbRuO$_3$ are metallic [2], and we have studied the pressure dependence of resistivity as shown in Fig. 1. At low pressures such as shown for 5 kbar there is a discontinuous hysteretic anomaly, coinciding with the first order structural phase transition. The discontinuity is not apparent at pressures above 10 kbar and the resistivities ρ. Fits to the resistivity data indicate an intriguing, low temperature electronic crossover at 60 kbar that is most probably the orbital transition being driven to $T \rightarrow 0$, where quantum critical orbital fluctuations are dominant.

To further elusidate how the the structural transition and both the Imma and Pnma structures of PbRuO$_3$ evolve with pressures above the 60 kbar, an angular dispersive diffraction experiment was carried out on ID09. The desired conditions were attained by loading polycrystalline PbRuO3 into a Diamond Anvil Cell (DAC) with a helium pressure transmitting medium and low temperaturese maintained by the insitu cryostat. Data were collected at 10, 15, 30, 50 and 125 kbar at a series of temperatures between 20 and 200 K at approximatly 20 K intervals. Supplementary data were collected up to 300 K.

The low temperature (<120 K) phases were identified as either Pnma or Imma structure, dependent on the presence of Pnma (h+k+l= 2n+)1 reflections and refined with the GSAS code. [3] Lattice parameters were extracted and a discontinuinty, clearly resolved in Fig. 2, ascribed to the phase transition was observed for the 10, 15 and 30 kbar datasets. Conversly the 50 and 125 K did not display any discontinuity which is direct evidence of the supression of the phase transition. The analysed high pressure-low temperature data is sumaried in the the phase diagram Fig. 3.

The results of this experiment show that the orbitally ordered phase of $PbRuO_3$ is suppressed at 55 kbar, in keeping with the electronic crossover observed in conductivity data. Further explorations of quantum critical phenomena around this suppressed transition are ongoing.

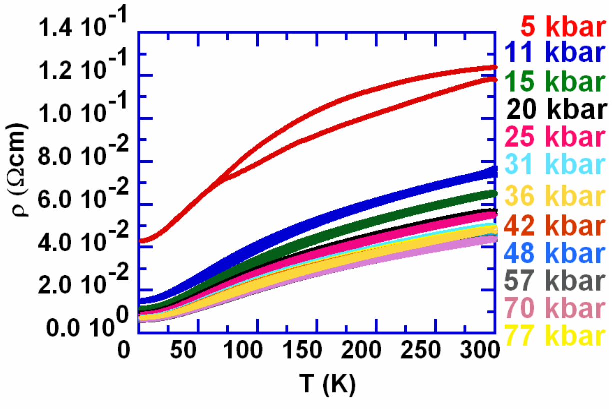

Fig. 1 Resistivity (ρ). The orbital ordering transition is evident from the bifurcation between cooling/warming data in ρ at 5 kbar.

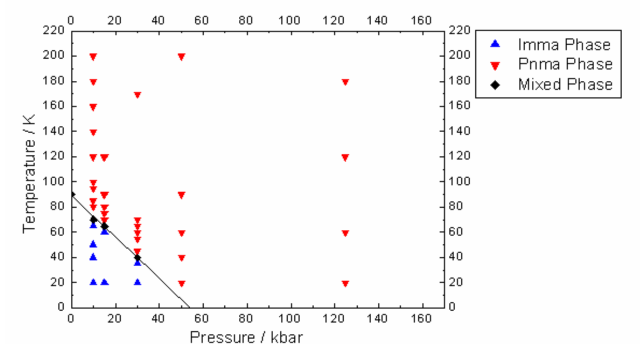

Fig. 3 Low temperature – high pressure phase diagram for $PbRuO_3$.

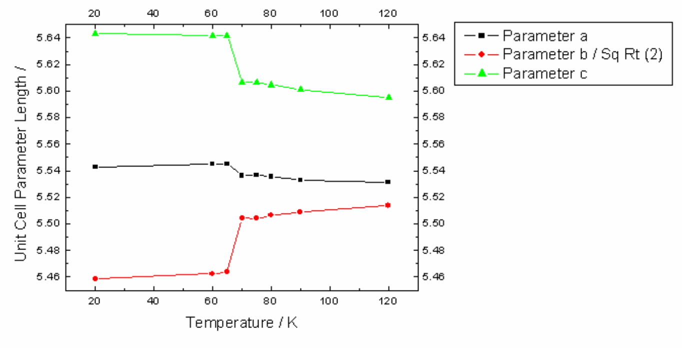

Fig. 2 Lattice paramenters as a function of tempearture at 15 kbar.

[1] S. A. J. Kimber, J. A. Rodgers, H. Wu, C. A. Murray, D. N. Argyriou, A. N. Fitch, D. I. Khomskii and J. P. Attfield, *Phys. Rev. Lett.*, **102**, 046409 (2009).

[2] Cheng JG, Zhou JS, and Goodenough JB *Phys. Rev.* B **80**, 174426 (2009).

[3] A.C. Larson and R.B. Von Dreele, "General Structure Analysis System (GSAS)", Los Alamos National Laboratory Report LAUR 86-748 (1994)