EUROPEAN **S**YNCHROTRON **R**ADIATION **F**ACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

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: Potassium and cesium study by Compton scattering under pressure: electronic s ¢ d transition	Experiment number: HS1377
Beamline: ID15B	Date of experiment: from: 02.10.2000 to: 11.10.2000	Date of report: 28.02.2001
Shifts: 24	Local contact(s): **Thomas Buslaps**	***Received at ESRF:***

Names and affiliations of applicants **(* indicates experimentalists):**
Christophe Bellin*
Amir Sabouri−Dodaran*
Wilson Crichton*

Report:

The alkali metals are of special interest in high−pressure physics particularly because of their aparently simple electronic structure with just one conduction electron outside the closed−shell configurations, which makes them specially interesting for comparison with different theoretical models. In case of heavy alkali metals such as cesium high pressure drives *s* −−> *d* transition. With increasing pressure Cs metal loose its nearly free−electron character and at sufficiently high density it essentialy become monovalent *d* transition metal.

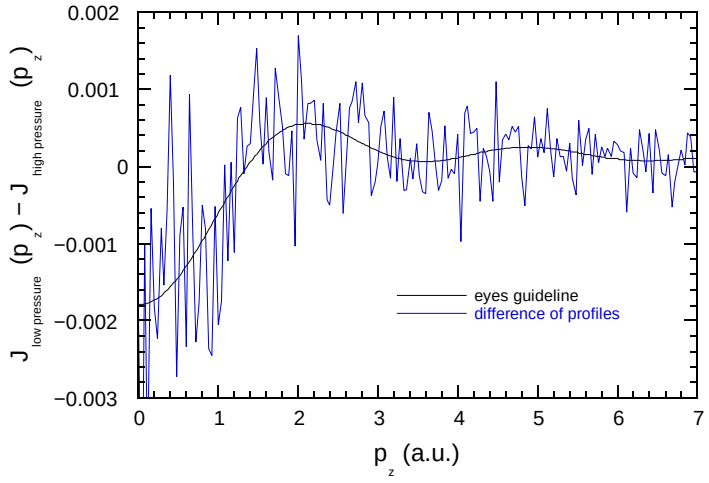
This transition is believed to be the driving force for destabilizing the common highly symmetric low−pressure cubic structures to lower symmetric structures. At ambient conditions all the alkali metals crystallize in the cubic−body−centered *cI2* structure type. Under pressure, the heavy metal cesium show phase transitions to fcc phase at 2.25 GPa [1−3], an isostructural fcc phase transition around 4.2 Gpa, a tetragonal phase after 4.4 Gpa and other phases which are out of the aim of our experiment.

Detailed experimental investigations of phase transitions in alkali metals have been performed for Cs [4] and Rb [5], as well as theoretical investigations for Cs [6 − 8]. In addition, using Mossbauer technique the electronic change was directly evidenced in case of Cs [9].

Compton scattering is particularly suitable for the study of the any change in the electronic density due to s −−> d transition since this method provides a direct probe of the ground−state electronic momentum density.

Two Compton profiles have been measured. The first measurement has been performed at the low pressure of 0.5 Gpa and the second at the high pressure of 5.5 GPA using the Paris−Edimburgh cell. This last pressure corresponds to the tetragonal Cs IV phase. The change of the pressure was followed by diffraction experiment in order to be able to control the input pressure on the sample. The experiment has been performed on ID15B using backscattered photons in order to obtain the Compton profile Compton profiles were measured by the way of a Ge−detector. The photons delivered by the synchrotron were monochromatized at the energy of 56 keV.

As shown in the figure below, the Compton profile measured at low pressure is lower at low momenta than the profile measured at high pressure. It means that the electronic density is more delocalized in momentum space in the case of the measurement performed at low pressure, i.e. more localized in charge space than the electronic density of Cs IV phase.



This experimental difference will be compared to theory. F. Mauri and A. Sabouri−Dodaran (LMCP, Paris) are performing *ab−initio* calculations in order to analyse the electronic density change due to pressure.

References:

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