ESRF

**Experiment title:**

X-ray absorption spectrometry of atoms with closed d-subshells

**Experiment number**:

HE-1522

**Beamline**:

BM29

**Date of experiment**:

from: April 10, 2003 to: April 14, 2003

**Date of report**:

August 25, 2003

*Received at ESRF:*

**Shifts:**

12

**Local contact(s)**: Dr. Gloria Subias Peruga

**Names and affiliations of applicants** (* indicates experimentalists):

***Alojz Kodre, Faculty of Mathematics and Physics, Jadranska 19, University of Ljubljana, SI-1001 Ljubljana, Slovenia**

***Iztok Arčon, Nova Gorica Polytechnic, Vipavska 13, SI-5000 Nova Gorica, Slovenija**

***Jana Padežnik Gomilšek, Faculty of Mechanical Engeneering, Smetanova 17, University of Maribor, SI-2000 Maribor, Slovenia**

***Andrej Mihelič, Institute Josef Stefan, Jamova 39, SI-1001 Ljubljana, Slovenia**

## Report:

In contrast to the experiment on Zn vapor from the previous year [1], the homologous Cd vapor is found considerably less agressive so that plain sealed steel cell and sealed quartz cell could be used to contain the vapor at the stable density. The fact may be attributed to the lower boiling point of Cd so that the cells could operate at a lower temperature. The best results were obtained by the quartz cell with 1 mm thick quartz windows.

The vapor density saturated above 900$^o$C, so that 950 $^o$C was chosen as a working point, with the resulting K edge jump of 1.8. Using the two-crystal fixed exit Si(311) monochromator, three identical runs of optimum quality were superposed to improve the signal to noise ratio.

After proper normalization and recalibration of the energy scale the absorption spectrum of Cd vapor is transformed into the atomic absorption background for use in the EXAFS analysis of cadmium compounds. The perfect match (Fig. 1) with the absorption spectrum of the cadmium metal foil measured in parallel with the vapor shows the excellent stability of the experiment. It is worth noting (inset) that the atomic backgrounds runs exactly along the middle of the EXAFS oscillations: with a properly measured atomic background there is no need for an artificial spline background currently used in EXAFS analysis packages. Moreover, the measured atomic background incorporates all the collective intraatomic effects, both the smooth extended fingerprints of the virtual excitations and the sharp features of the multielectron excitations.

Of the sharp multielectron features none are readily observable in the measured spectrum apart from the steep rise ~20 eV above the K edge. The apparent absence of the MPE is due to the large lifetime width of the K shell hole (7.3 eV) which smoothes out the sharp features. A best-fit model of the K edge profile, comprising the Rydberg series of the resonant transitions 1s -> np (n = 5, 6, ...) and the arctan profile of the excitation into the continuum, yields the width 7.3 eV convoluted with the 0.66 eV of the gaussian experimental resolution.

The existence of the MPE is best demonstated by the deconvolution of the natural width introduced recently by Filipponi [2] (Fig. 2). All the sharp features in the spectrum are found close to the Dirac-Fock estimates of the excitation energies. In the inset the atomic Cd edge resonance [1s]5p, not observed in any chemical species of Cd, is extremely strong, in the same vein as the edge resonance in the homologue Zn. (Publication is in preparation.)

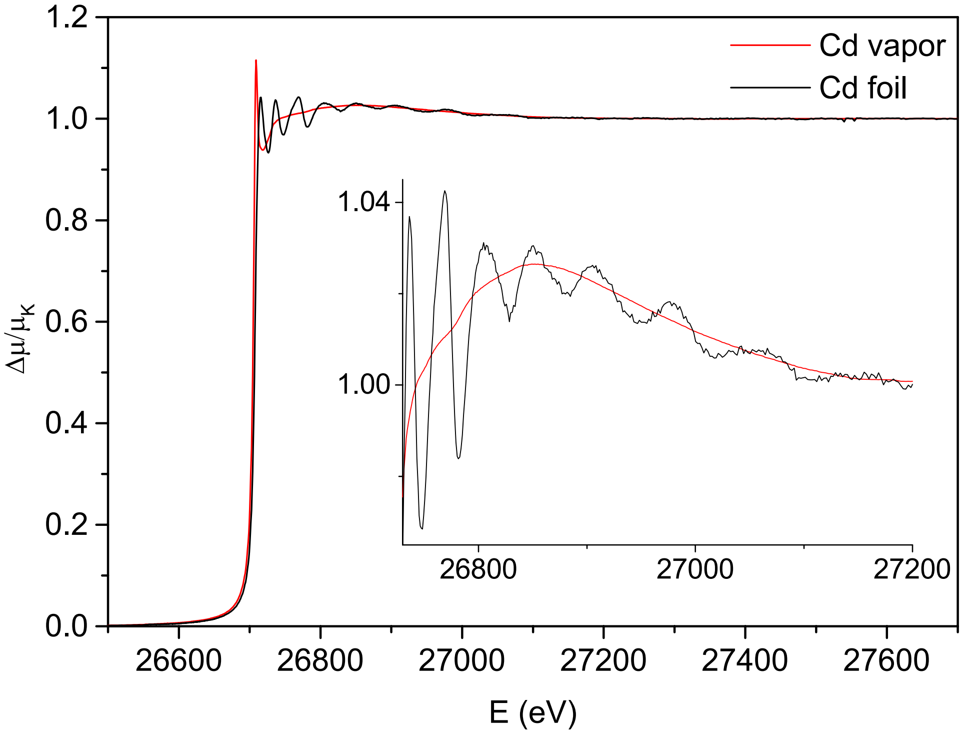

Fig. 1: The absorption spectrum of the Cd vapor as the atomic absorption background for the EXAFS spectrum of the Cd metal foil.

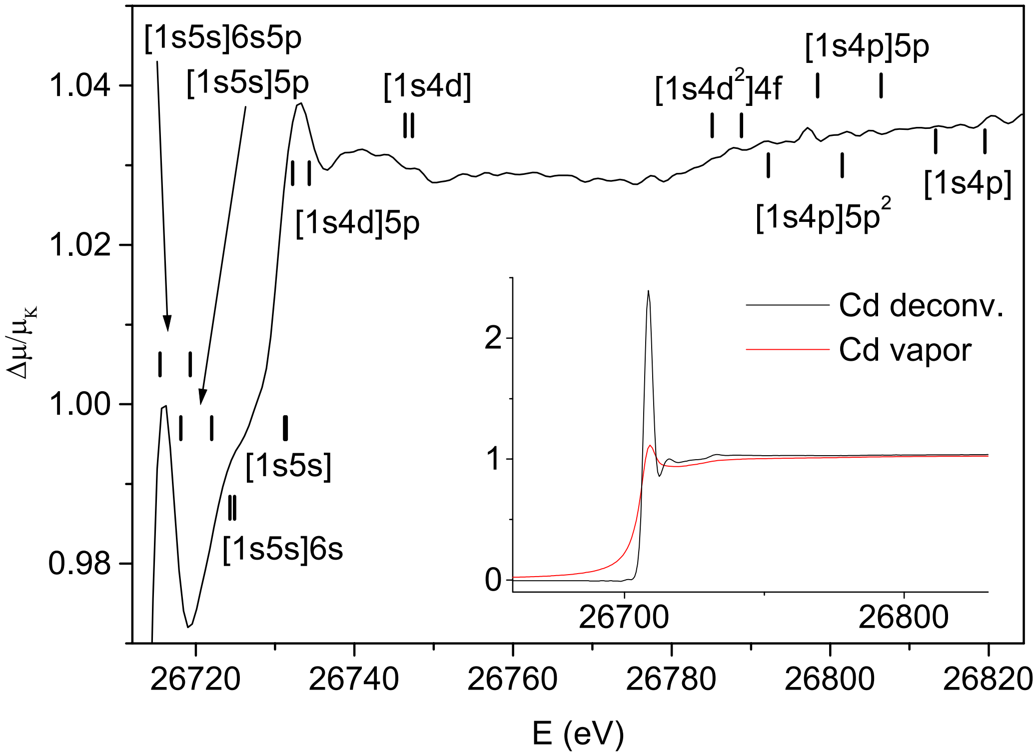

Fig. 2: The deconvolution of the Cd vapor absorption spectrum showing abundance of the multielectron excitation features indicated by vertical marks at their Dirac-Fock energies. The full size of the deconvoluted resonance at the edge is shown in the inset.

References:

1. Mihelič, A., Kodre, A., Arčon, I., Padežnik Gomilšek, J., and Borowski, M., Nucl. Instrum. Methods Phys. Res. B **196**, 194 (2002).

2. A. Filipponi, J. Phys. B **33**, 2835 (2000).