

**Experiment title:**The $K^h \beta$ Hypersatellites of Transition Metals**Experiment number:**

HE-790

Beamline:**Date of experiment:**

from: 14 April 2000

to: 21 April 2000

Date of report:

25 August 2000

Shifts:

24

Local contact(s):

J-P Rueff

*Received at ESRF:***Names and affiliations of applicants** (* indicates experimentalists):

*Moshe Deutsch, Bar-Ilan University, Israel

*Simo Huotari, University of Helsinki, Finland

*Keijo Hamalainen, University of Helsinki, Finland

Reut Diamant, Bar-Ilan University, Israel

Chi-Chang Kao, NSLS, BNL, U.S.A.

Report:

During this session we have measured the $K^h \beta$ hypersatellite spectra of Cr and Fe. After calibrating the emission energy scale using well-measured, strong diagram lines, we have measured for both materials the emission spectrum, the threshold energy for exciting the spectrum, and the cross-section evolution from threshold up. We have also measured the emission line intensity variation with incident energy of the calibration lines, which will serve as a transfer calibration for determining the hypersatellite-to-diagram spectral intensity ratio for each element.

The two spectra, background subtracted but otherwise raw, are shown in the Figure 1. As can be seen, the spectra show a complex underlying structure, indicating several overlapping lines. For a detailed analysis, ab-initio calculations are now being carried out to elucidate the details of the underlying structure. As can be seen from the initial fits of the calculated spectra (shown in a solid line) a reasonable fit can be obtained with the relativistic Dirac-Fock calculated spectra assuming only the main $1s^{-2} \rightarrow 1s^{-1}3p^{-1}$ transition, without contributions from any additional, higher-order transition. However, these are only preliminary conclusions at this stage.

The relatively low statistics, particularly for Cr, reflects the extremely low cross-sections for exciting these lines, 3-4 orders of magnitude relative to those of the diagram lines. Nevertheless, these, and our previous ID16-measured Mn $K^h \beta$ spectrum, are the only resolved $K^h \beta$ hypersatellites ever measured. The high, <1 eV, resolution will allow for an accurate determination from the spectra of the lifetime widths of the two-hole initial (KK) and final (KM) states involved. As observed, the Cr spectrum is significantly narrower than the Fe one. This is not only due to smaller lifetime widths in Cr, but also because the intensity of the $1s^{-2} \rightarrow 1s^{-1}3p^{-1}_{3/2}$ component relative to the $1s^{-2} \rightarrow 1s^{-1}3p^{-1}_{1/2}$ one is much smaller in Cr than in Fe. This is a

direct result of the evolution of the coupling from LS at small Z to intermediate at higher Z within the 3d transition elements.

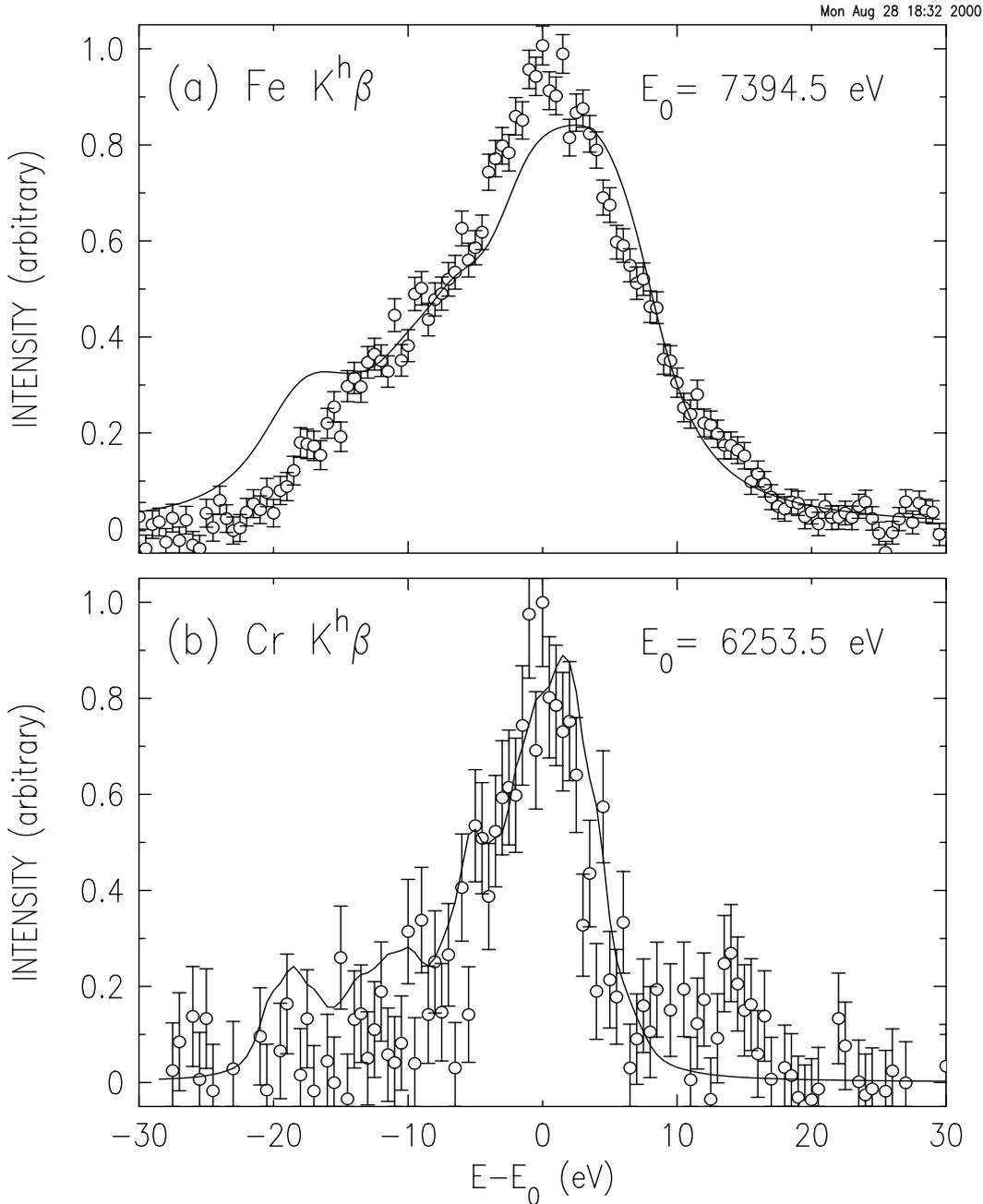


Fig. 1: Measured raw (a) Fe $K^h\beta$ and (b) Cr $K^h\beta$ hypersatellite spectra (points) and the fitted ab-initio Relativistic Dirac-Fock calculated spectra (lines).

These data, along with similar $K^h\beta$ spectra to be measured at ID16 and the $K^h\alpha$ spectra measured at ID16 and elsewhere, will be the first systematic study of the K hypersatellites for the 3d transition metals. They will shed light on the transition from the LS to jj coupling, occurring in this Z region (reflected in the relative intensities of the lines comprising the spectra), the Breit-Wigner interaction in these atoms (accessible through the line splittings and the shift of the hypersatellite spectra from the diagram ones) and intra-shell electronic correlations (contributing to the shifts from the diagram lines).