ESRF	**Experiment title:** Electronic Structure and Chemical Bonding in Distorted hcp Metals: Mg and Zn	**Experiment number**: HE-2136
Beamline: ID15B	**Date of experiment**: from: 05 April 2006 to: 11 April 2006	**Date of report**: 31 / 08 / 2007
Shifts: 18	**Local contact(s)**: Dr. Thomas BUSLAPS	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Prof. Dr. Wolf WEYRICH,* University of Konstanz, Germany

Prof. Dr. Martin JANSEN, MPI für Festkörperforschung, Stuttgart, Germany

Prof. Dr. Pekka SUORTTI, University of Helsinki, Finland

Dr. Jürgen NUSS,* MPI für Festkörperforschung, Stuttgart, Germany

Dr. Joachim TILLICH,* University of Konstanz, Germany

Report:

The experiments decribed here were performed as part of a joint project supported by the Deutsche Forschungsgemeinschaft (DFG) within the priority programme 'Experimental Electron Density as a Key to Understand Chemical Interactions'. The aim of this project is a deeper understanding of the anomalous crystal parameters of the elements Zn and Cd by investigating the electronic structure of these elements, and of Mg for comparison, in position an in momentum space using experimental as well as theoretical methods.

The high-energy inelastic x-ray scattering experiments were performed using the dispersion-compensating scanning spectrometer at beamline ID15B with an incident-photon energy of 89 keV [1]. Differently oriented plates of Zn and Mg were produced by spark erosion processing of single crystals grown by Bridgman technique (MaTecK, Jülich). The face of the plates was 7 mm high and 3 mm wide. The thickness of the Zn specimens was 0.7 mm, that of the softer Mg samples 1 mm. The surface normals were chosen to coincide with (or to come close to) the directions from a reference atom to its neighbours with increasing distance (Fig. 1a): R1 [423] (nearest interplanar neighbour), R2 [100] (nearest intraplanar neighbour), R3 [001], R4 [10,2,3]; R5 [210] and R6 [101] (Mg only). Owing to the preparation procedure, the surfaces of the samples were rather rough and corroded. In conjunction with the low penetration depth of the mapping X-rays in backscattering with a laboratory sealed-tube system, particularly some Zn Laue diagrams were so diffuse and distorted that no reliable sample orientation could be achieved. Therefore part of the beam time had to be used to measure high-energy oscillation diagrams in transmission, which fortunately revealed a very satisfactory crystallographic quality of the bulk part of the samples. Only in the case of the Zn sample for direction R2, a misorientation was detected that was so large that the desired direction was inaccessible by compensating sample rotations without serious deterioration of the Compton scattering spectrum. In order to obtain the Compton profile for this direction, the R4 sample was used, rotated by 47° around its vertical [120] axis. However, because of this excessive rotation, the recorded data suffer from multiple-scattering distortions and are therefore not satisfactory.

The resolution of the spectrometer was determined for each direction by analysing the elastic line being recorded together with the Compton profile. The values of the resolution function at the Compton peak were

in the range of 0.13–0.16 p_0 for Mg and 0.12–0.16 p_0 for Zn. The processed experimental Compton profiles are normalised to the number of electrons per formula unit (Mg: 12, Zn: 30). Differences of the directional Compton profiles clearly show the anisotropy of the momentum density, in Zn as well as in Mg. As examples we present the differences between R1 and R3 for Zn (Fig. 1c) and for Mg (Fig. 1d). Although we had to compromise on the statistics because of the high number of directions and the limited beam time, it has yielded the first certain observation of the small anisotropy of the electron momentum density of Mg as well as the corresponding first fully resolved anisotropy for Zn, both due to the significantly improved performance of the dispersion-compensating scanning spectrometer [1] at ID15B. Both anisotropies agree well with earlier theoretical APW (Mg, [2]) and KKR (Zn, [3]) and our recent Hartree–Fock [4] calculations, resp., showing, however, also quantitative deviations owing to the various approximations in the theoretical approaches. In particular, in comparison to the Hartree–Fock results the measured anisotropy of the momentum density in Zn is much larger than the one in Mg.

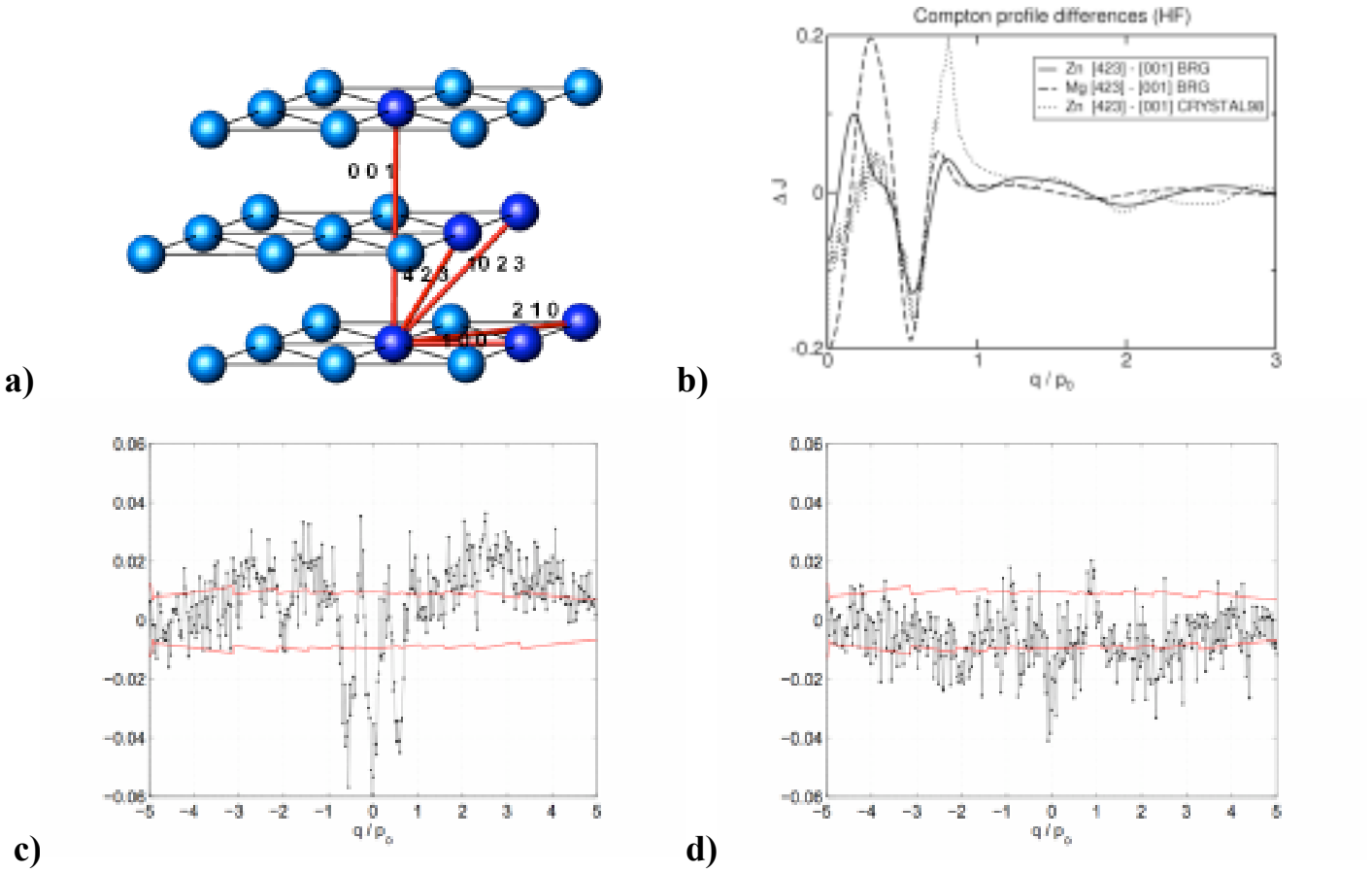

Figure 1: **a)** Directions of the scattering vector in position space. **b)** Differences of directional Compton profiles ([423] – [001]) computed at the Hartree–Fock level either via Fourier transformation of the reciprocal form factor $B(\mathbf{s})$ (program BRG) or by integration of the momentum density (program CRYSTAL98). **c)** and **d)** Differences of measured directional Compton profiles ([423] – [001]) of Zn (c) and Mg (d).

Measurements on the two next-neighbour directions [423] and [100] (for Zn so far distorted by multiple scattering) with substantially better statistics, both for Mg and Zn, are planned as the next necessary step of this investigation.

References

[1] N. Hiraoka, T. Buslaps, V. Honkimäki, P. Suortti, J. Synchrotron Rad. **12**, 670 (2005).
[2] S. Wakoh, J. Phys. Soc. Jap. **50**, 490 (1981).
[3] H. Reniewicz, A. Andrejczuk, L. Dobrzynski, E. Zukowski, S. Kaprzyk, J. Phys.: Condens. Matter **13**, 11597 (2001).
[4] U. Wedig, M. Jansen, B. Paulus, K. Roskiszewski, P. Sony, Phys. Rev. B **75**, 205123 (2007).