ESRF	**Experiment title:** Temperature dependent Magnetic EXAFS at Gd L-edges in Gd metal and in GdZn intermetallic compound	**Experiment number**: HE-536
Beamline: ID 12 A	**Date of experiment**: from: 16.6.1999 to: 21.6.1999	**Date of report**: 25.2.2000
Shifts: 15	**Local contact(s)**: A. Rogalev	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Heiko Wende*, Fabrice Wilhelm*, Panagiotis Poulopoulos*, Klaus Baberschke
Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin

Thomas A. Lograsso, Deborah L. Schlagel
Ames Laboratory, Iowa State University, Ames , Iowa USA 50011

Report:

Following the suggestion of the review committee we carried out the temperature dependent magnetic EXAFS (MEXAFS) experiments at a Gd single crystal first. The data were taken at four temperatures (10K, 100K, 200K and 250K) at the L_3, L_2, and L_1-absorption edges using the gap-scanning as well as the fixed-gap setup of the beamline. As the gap-scanning technique worked very satisfactorily the detailed investigations were carried out with a moving gap to keep the degree of polarization constant for the full photon energy range of ΔE=1200 eV. Using this setup we were able to record MEXAFS data of high quality as shown in Fig. 1 for the Gd L_3-edge (for the sake of a better comparison, the data for 200K are not presented in this figure). The MEXAFS oscillations $\chi_M(k)$ can be detected up to a photoelectron wavenumber of k=13.0 $Å^{-1}$. A clear temperature dependent damping can be seen also in the corresponding Fourier transforms of the MEXAFS oscillations as given in Fig. 2. One origin of this damping is the reduction of the magnetization as T=250 K corresponds to a reduced temperature of $T/T_c \approx 0.85$. The reduction of the magnetization will lead to a simple scaling of the MEXAFS oscillation by a factor. But there is an additional type of damping which is Debye-Waller factor like ($e^{-2\sigma^2 k^2}$) and hence leads to an exponential damping in the magnetic EXAFS. This can be seen from the fact that the MEXAFS oscillations at 250K are only reduced by 50% of the 10K data in the low k-range (k=2.5 $Å^{-1}$ to k=9.0 $Å^{-1}$) whereas the oscillations are nearly completely damped for the higher k-values starting from k=9.0 $Å^{-1}$. This indicates that lattice vibrations influence the spin dependent scattering potential leading to an additional reduction of the MEXAFS signal as it

is also found for the regular EXAFS in our experiment. The analysis of the temperature dependence of the normal EXAFS reveals that the temperature dependent damping due to

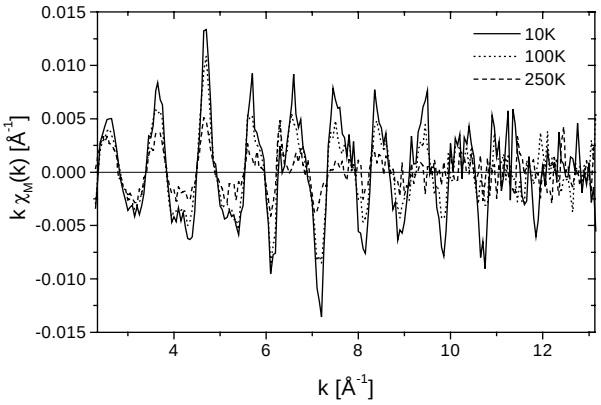

Fig. 1: Temperature dependent MEXAFS oscillations k χ_M(k) for a Gd single crystal at the L_3 absorption edge versus the photoelectron wavenumber

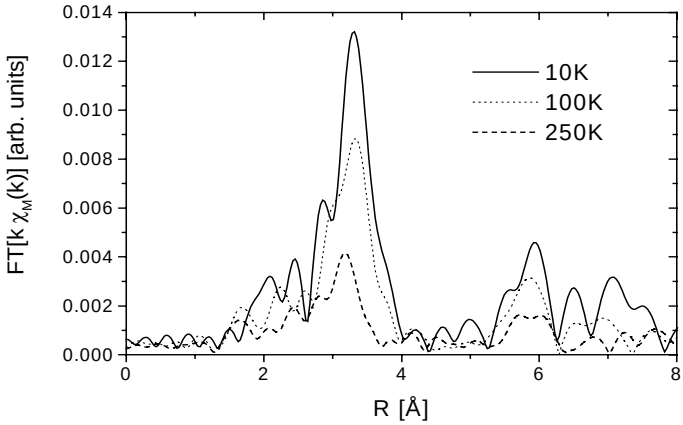

Fig. 2: Fourier transform FT[k χ_M(k)] of the MEXAFS oscillations given in Fig. 1.

thermal vibrations is described by a Debye temperature of θ_D=160 K. This shows that the data recorded at 250 K are strongly damped due to thermal vibrations. This must be taken into account when analyzing the local magnetic fluctuations in detail. We carried out *ab initio* calculations in order to separate the multiple- from the single-scattering contributions for the normal EXAFS and the magnetic EXAFS signal. It turns out that the consideration of the multiple-scattering paths is essential to describe the fine structure of the MEXAFS and the MEXAFS [1]. Given in Fig. 3 is the comparison of the experimental EXAFS data with the *ab initio* calculation (FEFF7) which includes multiple- and single scattering paths. The good agreement between theory and experiment enables us to analyze the temperature dependence of the individual scattering paths. This work was presented as an invited talk at the 'Workshop on Theory and Computation for Synchrotron Radiation' held in Frascati (Italy) in September 1999 [1]

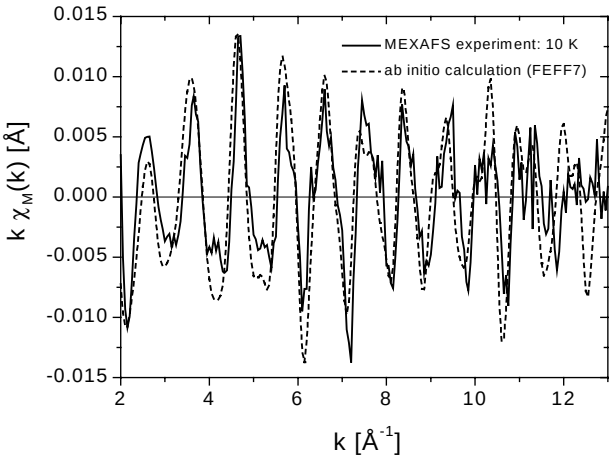

Fig. 3: Comparison of the experimental MEXAFS data at 10K to an *ab initio* calaculation (FEFF7). The phase as well as the enveloping amplitude is well reproduced by the calculation.

[1] H. Wende, F. Wilhelm, P. Poulopoulos, K. Baberschke, J.W. Freeland, Y.U. Idzerda, A. Rogalev, D.L. Schlagel, T.A. Lograsso, and D. Arvanitis: *On the Temperature Dependence of Multiple- and Single-Scattering Contributions in Magentic EXAFS*, proceedings (in print) of the 'Workshop on Theory and Computation for Synchrotron Radiation' held in Frascati (Italy) in September 1999