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- 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:** Diffraction anomalous fine structure measurements of ferromagnetic inclusions in semiconductor layers	**Experiment number**: **SI- 1841**
Beamline: BM02	**Date of experiment**: from: 17. 6. 2009 to: 23. 6. 2009	**Date of report**: 13. 8. 2009
Shifts: 18	**Local contact(s)**: Dr. Hubert Renevier	*Received at ESRF:*

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Report:

Ferromagnetic semiconductor composites containing ferromagnetic small inclusions in a diamagnetic semiconductor matrix represent a very promising route for a fabrication of semiconductor ferromagnetic systems with the Curie temperature above 300 K. Among a broad variety of these systems, Ge(Mn) attracted a lot of attention nowadays, since the nucleation and growth of ferromagnetic Mn_5Ge_3 inclusions in Ge(Mn) can be easily controlled during the molecular-beam epitaxy (MBE) growth by changing the deposition temperature. A series of papers [1-3] has been devoted to the investigation of the magnetic properties of Ge(Mn) and to the determination of the crystal structure of the precipitates by transmission electron microscopy and electron diffraction. In our previous papers [4,5] we have used grazing-incidence (GID) and coplanar x-ray diffraction for the measurement of the size of the precipitates and for the study of elastic strains in Ge matrix around the precipitates. We have also found that the Mn_5Ge_3 hexagonal lattice exhibits few possible orientations with respect to the cubic host crystal; the mutual orientation of these lattices (topotactical relation) for the precipitates buried at the substrate surface differs from that of the precipitates placed close to the free layer surface.

The crystal structure of the Mn_5Ge_3 precipitates has been determined from selected-area electron diffraction in transmission electron microscopy and confirmed by x-ray diffraction. These measurements revealed that the precipitates contain hexagonal lattice with the space group P63/mcm (193) [1], however the experimental data obtained so far did not allow to determine exact positions of the atoms in small precipitates with a necessary accuracy. For the determination of the positions of atoms in crystalline or nano-crystalline materials, EXAFS is the method of choice. In our case however this method is not applicable, since Mn atoms are present not only in the precipitates, but also diluted in the Ge host lattice, and it is impossible to distinguish the contributions of these two atom types to the total EXAFS signal. We used the DAFS method instead (diffraction anomalous-fine structure), in which the diffracted intensity is measured in a given point $\boldsymbol{Q}$ in reciprocal space as a function of the photon energy around the MnK absorption edge.

We have investigated a series of Ge(Mn) layers deposited by MBE on Ge(001) substrates, the layer thickness was 100 nm and the samples differ in the nominal Mn amount and in the deposition temperature. The details of the sample growth and the GID data measured on these samples are presented in Ref. [4]. The DAFS measurements have been carried out at the BM02 beamline at ESRF. We measured the energy dependence of the intensity diffracted in the grazing-incidence geometry, and we chose the position $\boldsymbol{Q}$ close to the in-plane diffraction maximum 300 of the hexagonal lattice, and in the maximum of the layer peak (the in-plane

diffraction 220 of the cubic Ge lattice). The incidence angle α_i of the primary radiation was chosen 0.3 deg, i.e., close to the critical angle of total reflection. The diffracted radiation was measured by a linear detector vantec perpendicular to the sample surface, and for the evaluation we use the signal integrated over all ext angles α_f.

From the measured energy dependences of the diffracted intensity we have determined the real and imaginary parts $\chi'(k)$ and $\chi''(k)$ of the oscillating (EXAFS) parts of the atomic form-factor of Mn using an iteration procedure and Kramers-Kronig integrals [6,7]. The numerical treatment consisted in the following steps:

1. We fitted the measured energy dependence of the diffracted intensity $I(E)$ to a smooth function $I_s(E)$ (polynomial fit) above the edge energy, i.e. for $E>E_K$, and we calculated the relative difference

$$\Psi(E) = [I(E) - I_s(E)]/ I_s(E).$$

The function $\Psi(E)$ equals the relative difference of the squares of the structure factors

$$\Psi(E) = [|F(E)|^2 - |F_s(E)|^2]/ |F_s(E)|^2,$$

where F is the structure factor of the Mn_5Ge_3 lattice including the oscillatory part $\chi'(E) + i\chi''(E)$ of the Mn atomic form-factor, and F_s is the same structure factor without the oscillatory part.

2. We assumed $\chi''(E) = 0$
3. We calculated $\chi'(E)$ from the experimentally determined function $\Psi(E)$ and from $\chi''(E)$.
4. We calculated $\chi''(E)$ from $\chi'(E)$ numerically using the Kramers-Kronig integrals [8,9].
5. We repeated the steps 3, 4 until a convergence is reached.
6. We converted the resulting dependences $\chi'(E)$, $\chi''(E)$ to $\chi'(k)$, $\chi''(k)$, where k is the length of the wave vector of the photoelectron: $k = \sqrt{2m(E - E_K)}/\hbar$.
7. We calculated the Fourier transformations $\chi'(R)$, $\chi''(R)$ to real space.

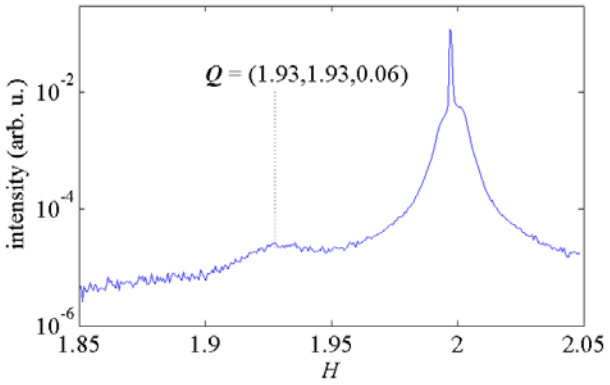

Fig. 1 Radial scan of sample R1626F taken at E = 6.8 keV and α_i = 0.3 deg; the vertical line denotes the position, where the DAFS scan was taken.

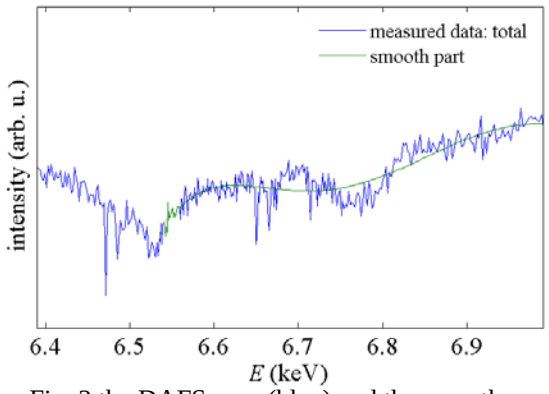

Fig. 2 the DAFS scan (blue) and the smooth polynomial; fit (green)

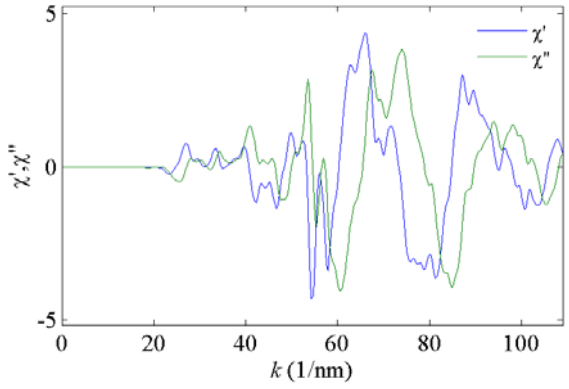

Fig. 3 The functions $\chi'(k)$, $\chi''(k)$ obtained by the iteration procedure

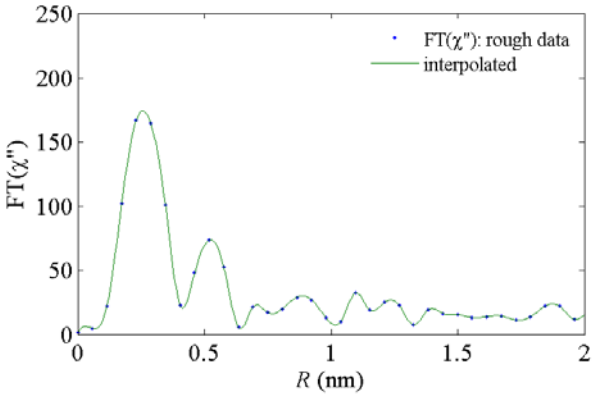

Fig. 4 The Fourier transformation of χ'' into real space

As an example, we present here the results measured in sample R1626F (3.4% Mn, deposition temperature 120°C). Figure 1 shows a radial GID scan taken around the in-plane diffraction Ge(220) for E = 6.8 keV. In

the position denoted by the vertical line in Fig. 1 we measured the DAFS scan plotted in Fig. 2 along with its smooth fit. The results of the iteration procedure described above are plotted in Fig. 3 and the Fourier transformation $\chi'(R)$ of $\chi'(k)$ into real space is shown in Fig. 4. The maxima of this function correspond to the distances of the absorbing Mn atom in the Mn_5Ge_3 precipitates to its neighbors (the radii of the first coordination spheres).
We are going to simulate the functions $\chi'(k)$, $\chi''(k)$ ab-initio using the program FDMNES [10] and compare the simulated curves with the measurements. From this comparison we will determine the bond lengths of the absorbing Mn atom to its neighbors.

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