# Temperature dependent EXAFS study of $Mn_5Si_3C_x$

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The intermetallic compound $Mn_5Si_3$ exhibits antiferromagnetic order at temperatures below 100 K. The magnetic transition is accompanied with an orthorhombic distortion of the hexagonal unit cell [1]. Further structural and magnetic analysis on single-crystalline samples have shown that a second antiferromagnetic transition occurs at 66 K together with a change of the *c* axis dimension [1]. Remarkably, the antiferromagnetic $Mn_5Si_3$ becomes ferromagnetic by doping with carbon [2]. For $Mn_5Si_3C_x$ films prepared by magnetron sputtering on at substrate temperatures of $T_S$ = 740 K a maximum Curie temperature of $T_C$ = 350 K was found for $x \approx 1$ and the local magnetic Mn moments were determined by zero-field NMR measurements [3, 4]. Earlier structural investigations performed at room temperature provided strong evidence that the carbon is incorporated in the octahedral voids of the hexagonal $D8_8$ structure (space group $P6_3/mcm$) surrounded by Mn atoms [5]. However, it is not clear whether or not a structural phase transition occurs below room temperature similar to the parent $Mn_5Si_3$ compound. In this respect, conventional x-ray powder diffractometry is an inadequate method to check for a small orthorhombic distortion, since only the peak intensities are slightly changed which are furthermore reduced by the film texture. Therefore, we have started an extended x-ray absorption fine structure (EXAFS) study on $Mn_5Si_3C_x$ to investigate the local structural properties in detail. A previous EXAFS study performed at ambient temperature suggested a change of the local Mn environment by the incorporation of carbon in the octahedral voids [4]. However, a detailed analysis of the data in terms of a multiple scattering approach by FEFF6 code was not successful and was presumably hampered by the large thermal attenuation of the EXAFS oscillations.

200-nm thick polycrystalline $Mn_5Si_3$ and $Mn_5Si_3C_{0.75}$ films were prepared by magnetron sputtering on (1-102)-oriented sapphire substrates at a substrate temperature $T_S$ = 740 K. In addition, an $Mn_5Si_3$ powder sample was prepared by sintering a mixed powder of the elemental constituents at 1170 K for eight days for comparison with the $Mn_5Si_3$ film. X-ray absorption spectra at the Mn K-edge were taken at photon energies 6400 – 7500 eV at beamline A1 in the two-crystal mode using a Ge fluorescence detector. Contribution due to the Fe *K* fluorescence radiation from the background was minimized by electronic discrimination of the Ge detector signal. Multiple EXAFS scans were taken at temperatures $T$ = 5 K, 82 K, and 150 K employing a liquid He flow-cryostat. All spectra were calibrated with an Mn foil (*K*-edge at 6537.7 eV) and were corrected for self-absorption effects according to Ref. [6] prior to further data processing. The obtained EXAFS oscillations $\chi(k)k^3$ were Fourier transformed into R space by application of a Bessel window.

Fig. 1 shows the Fourier transforms FT ($\chi$ $k^3$) of the different $Mn_5Si_3C_x$ samples at various temperatures $T$. For $T$ = 150 K all FT show a similar behavior indicating a similar short range order around Mn in the hexagonal $D8_8$ structure. This is also observed for $T$ = 82 K indicating that the orthorhombic distortion of the crystallographic *a* and *b* axes reported for single-crystalline samples [1] is very small in the investigated polycrystalline samples. In contrast, the data measured at $T$ = 5 K exhibit clear differences when comparing the FT of the films with the FT of the powder sample, in particular around R = 3.7 Å. However, the qualitative behavior of FT(R) of the films seems to be independent of temperature. This demonstrates that the films exhibit do not exhibit an orthorhombic distortion - even not for the undoped $Mn_5Si_3$ film - in contrast to the bulk $Mn_5Si_3$ powder sample. Moreover, the local structural order of $Mn_5Si_3$ films is similar to $Mn_5Si_3C_{0.75}$ films. For a more detailed analysis the experimental data should be compared with the FT derived from a theoretical calculation of the EXAFS signal by a multiple scattering approach using FEFF6 code [7]. Preliminary calculations have been performed for the films, see Fig. 1. For this purpose we have used the lattice parameters measured by x-ray diffraction at $T$ = 25 K assuming a hexagonal $D8_8$ structure. Thermal broadening was taken into account by application of the Debye model with a Debye temperature $\theta_D$ = 400 K. The agreement between the experimental data at $T$ = 5 K and the FEFF calculation is very good for the $Mn_5Si_3$ film whereas for the carbon doped $Mn_5Si_3C_{0.75}$ film differences are found around R = 3.8 Å. Further data analysis is necessary to refine the structural parameters by successive fitting the theoretical FEFF calculations to the experimental data.

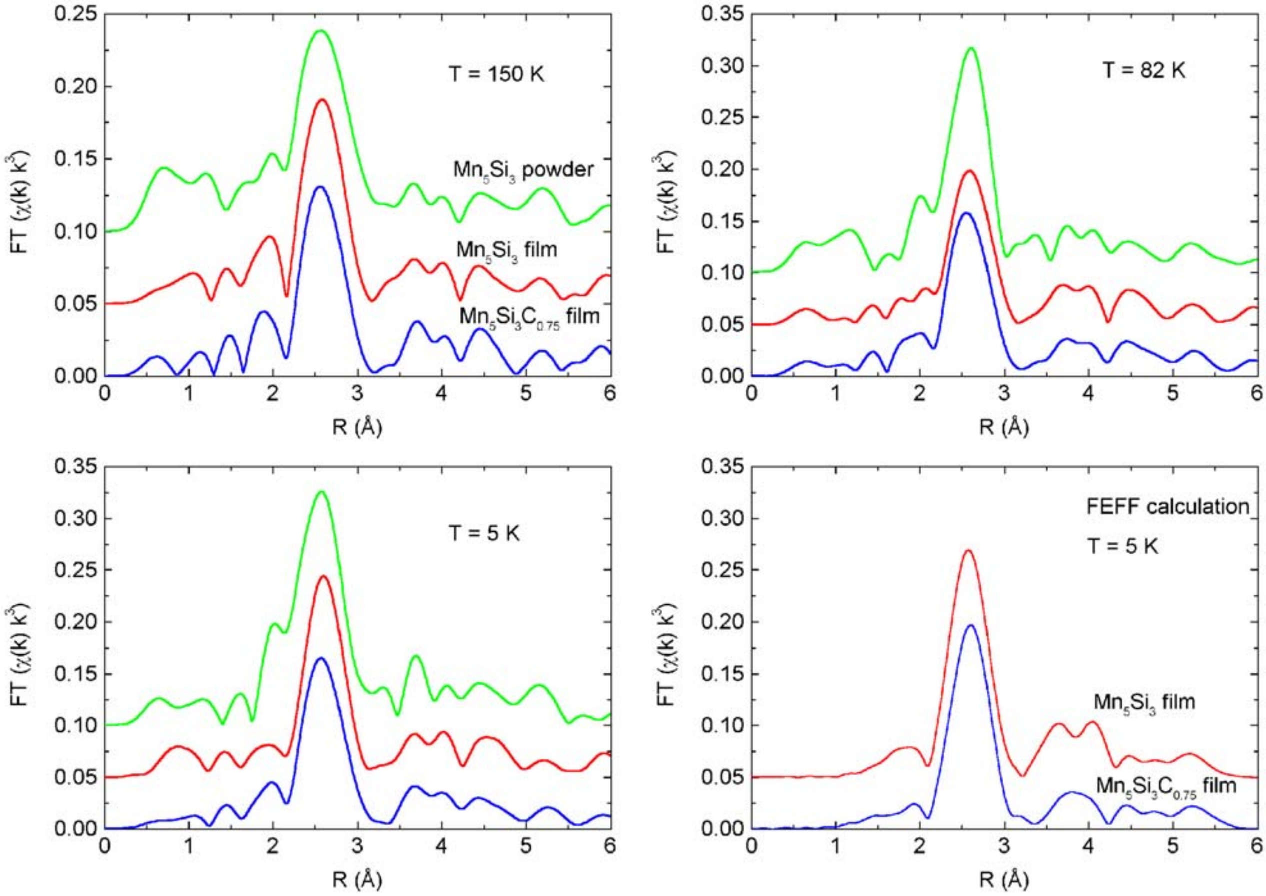

Figure 1: Fourier transforms of the Mn *K*-edge EXAFS oscillations $\chi$(k)k$^3$ for different $Mn_5Si_3C_x$ samples at various temperatures *T*. In each panel the upper two curves are successively shifted upward by 0.05 for clarity. Also shown are the transforms for $Mn_5Si_3$ and $Mn_5Si_3C_{0.75}$ at $T = 5$ K derived from a multiple scattering calculation of the EXAFS signal using FEFF6 code.

## References

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