Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information :

Atomic layer doping of Mn magnetic impurities from surface chains at a Ge/Si hetero-interface

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Absorption spectra of Mn δ-doped layer

XAFS measurements were performed at the Mn K-edge in N_2 at the beamline BL37XU, in SPring-8. The X-rays from the undulator source were monochromatized by a Si(111) double-crystal monochromator. The incident X-ray intensity was measured by an ionization chamber. The XAFS spectra were measured in the wavelength dispersive fluorescence mode using a 19-element Ge solid state detector. The sample was mounted on a swivel stage to set the incident angle between the X-rays and the sample surface at 4°. The measurement direction was defined by two angles, ϕ and θ, between the electric field vector $\boldsymbol{E}$ and the Mn atomic chain. ϕ is the in-plane angle, such that $\phi = 90°$ when $\boldsymbol{E}$ is perpendicular to the Mn chain, and 0° when parallel. θ is the out-of plane is angle, such that $\theta = 0°$ when $\boldsymbol{E}$ is perpendicular to the sample normal. The XAFS spectra were analyzed using the Demeter software.[1] The obtained X-ray absorption near-edge (XANES) spectra are shown in Fig. 1 and are similar to previous results.[2,3] There is a clear difference between the Si and Ge capped samples in the vertical direction.

Fitting with one-shell Mn-Ge model

Curve fitting with a one-shell model for Mn-Si and Mn-Ge was applied to the Ge capped sample. Theoretical scattering phase shifts and amplitudes were calculated using FEFF8.[4] The obtained distances (R), effective coordination numbers (CN*), Debye-Waller factors (σ^2), relative error between the fit and data (R-factor) and an energy shift parameter ΔE, used to align the theoretical spectrum to the measured spectrum, are listed in Table 1. Since many of the parameters show large deviations, these fitting results are not reliable.

Reference : powder samples

As a reference, a Mn crystal and several Mn silicide and germanide powders diluted in BN powder were characterized by XAFS measurement. The X-ray absorption fine structure and

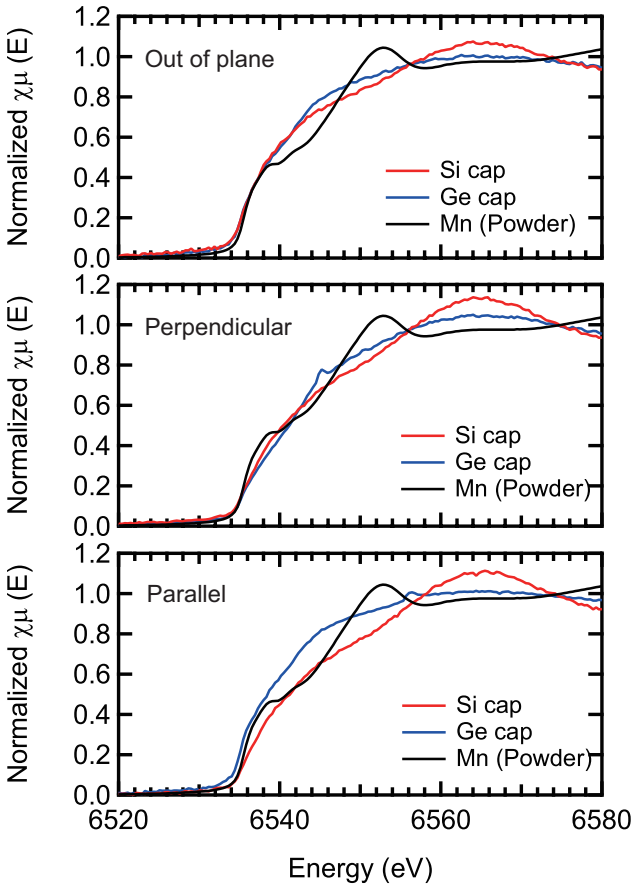

Figure 1: Normalized absorption spectra of Mn δ-doped samples capped by Si and Ge. Spectra were obtained in three different directions, out-of-plane ($\phi = 0°,\ \theta = 0°$), perpendicular ($\phi = 90°,\ \theta = 90°$) and parallel ($\phi = 0°,\ \theta = 90°$).

Fourier transforms at $k = 2 - 12$ Å^{-1} of the Mn K-edge EXAFS spectra of these samples are shown in Fig. 2 and Fig. 3, respectively.

Table 1: Structural parameters for the Mn-Ge nearest neighbor shell obtained from curve fitting analysis of the Mn K-edge EXAFS spectra of a Ge capped Mn δ-doped layer for $2 < k < 10$ Å^{-1}. Mn-Si oscillation is dominant and CN^* is dependent on the measurement geometry, which is based on structural anisotropy. ΔE (eV) and R-factor represent the energy shift to align theoretical spectrum to the measured spectrum and the relative error between the fit and data.

Samples	R (Å)	CN^*	σ^2 (Å^2)	ΔE (eV)	R-factor
Mn-Ge (out-of-plane)	2.3 ± 0.1	-3 ± 6	0.01 ± 0.02	0	0.02187
Mn-Ge (perpendicular)	2.3 ± 0.2	-5 ± 11	0.01 ± 0.02	-1.7	0.03285
Mn-Ge (parallel)	2.4 ± 0.2	5 ± 15	0.02 ± 0.03	-19	0.03261

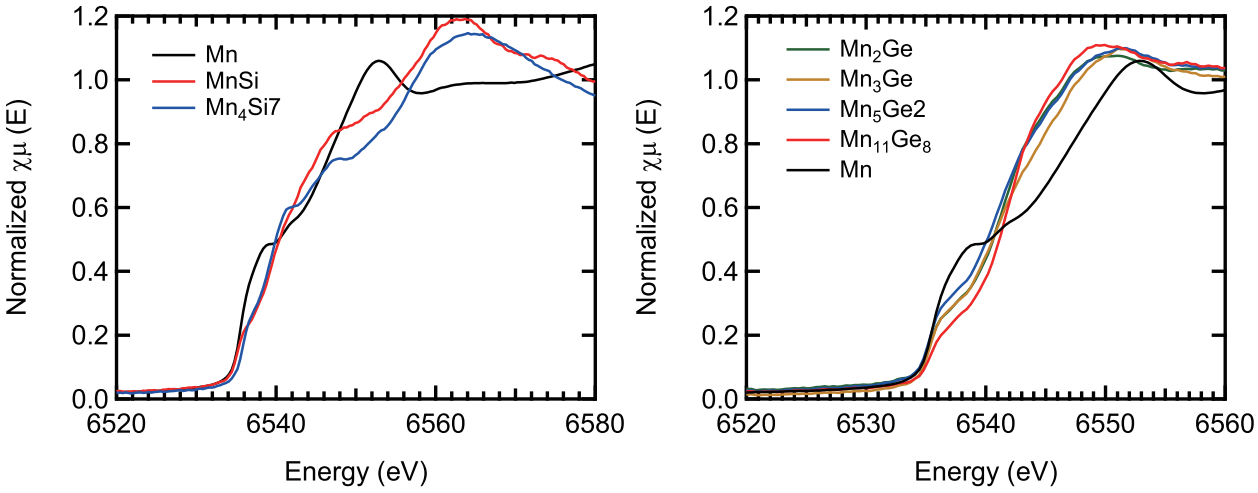

Figure 2: Normalized absorption spectra of Manganese (a) Silicide and (b) Germanide

References

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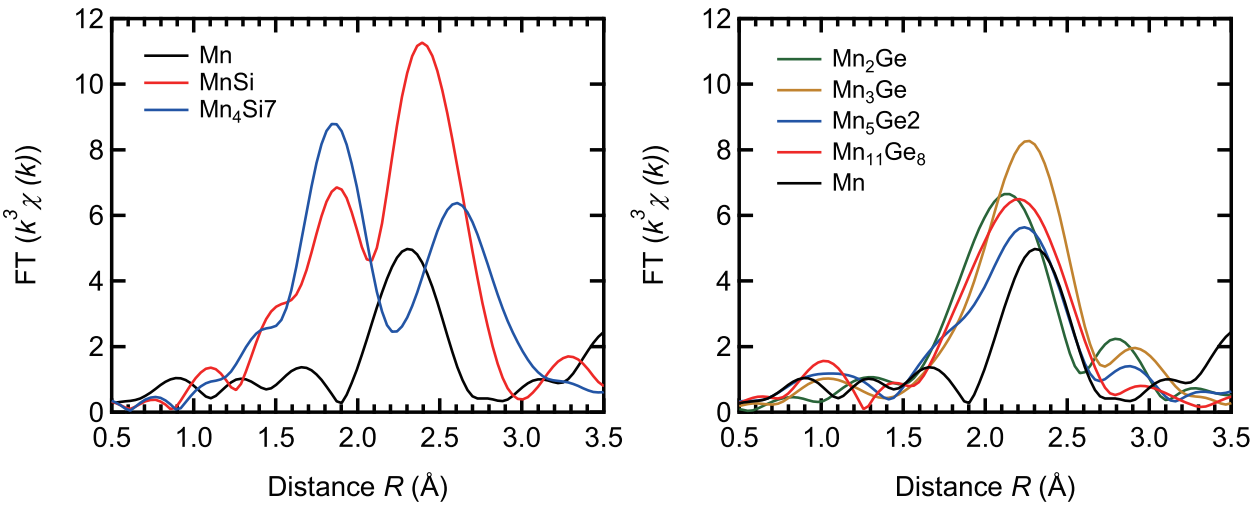

Figure 3: Fourier transform at $k = 2 - 12$ Å^{-1} of Manganese (a) Silicide and (b) Germanide