

Report of Experiment 25-01-794

“The influence of MnN_x in the electrical and optical properties of Si_3N_4 : XAS study at the Mn K-edge”

Experimental: XANES and EXAFS ($k = 12$) in fluorescence detection mode. Angle x-ray beam-detector of 90° ; beam-sample 30° aprox.

Measured samples:

- Mn foil (transmission)
- $[MnN_x(1.5 \text{ nm})/Si_3N_4(3\text{nm})]_{10}$ samples with P_{N_2}/P_{total} ratio of: 0%, 25%, 50%, 75%, 100% (20 bilayers) and also Mn/ Si_3N_4 (1 Mn layer with 3nm of Si_3N_4 on top, named as MnSN0)

The normalized sample spectra are shown in Fig. 1.

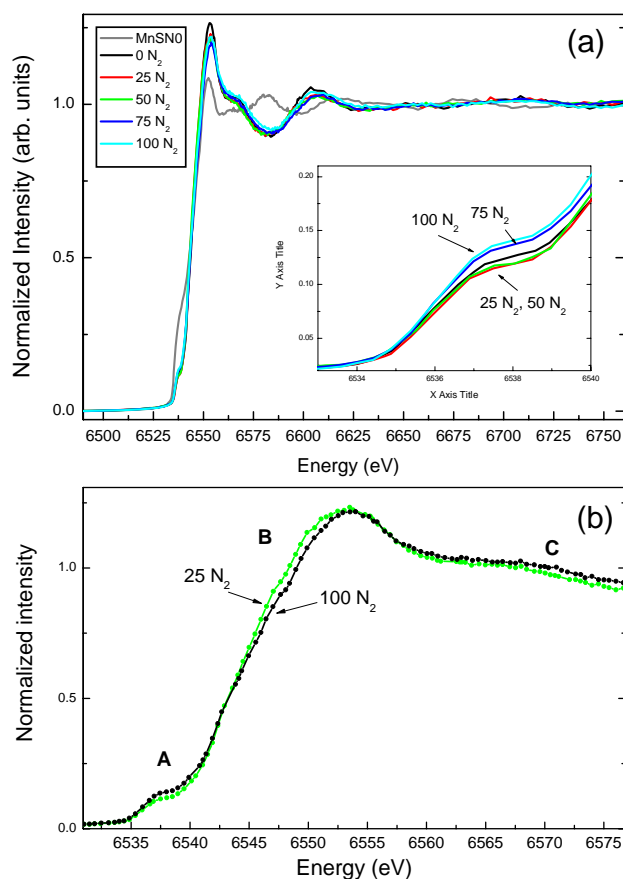


Fig. 1. Normalized sample spectra. A zoom of the pre-peak region is shown in the inset of Fig1 (a). Fig 1(b) exhibits the differences between $[MnN_x(1.5 \text{ nm})/Si_3N_4(3\text{nm})]_{10}$ samples with P_{N_2}/P_{total} ratio of 25% and 100 %.

First analysis shows that, except for MnSN0 sample, with mostly metallic Mn, just slight differences appear in the XAS spectra of $[\text{MnN}_{x(1.5 \text{ nm})}/\text{Si}_3\text{N}_{4(3\text{nm})}]_{10}$ samples prepared with different $P_{\text{N}_2}/P_{\text{total}}$ ratio.

The XANES region of $[\text{MnN}_{x(1.5 \text{ nm})}/\text{Si}_3\text{N}_{4(3\text{nm})}]_{10}$ sample prepared with 0% of N_2 (black line) presents some differences respect to the others, as enhanced white line intensity, increased XAS features amplitude and different evolution of the pre-peak intensity in comparison with the other samples from the series, as it can be observed in Fig 1(a).

Despite the slight differences, a direct relation seems to appear between the optical and electrical properties of the samples series and their XAS spectra. Clear differences can be observed in the pre-peak intensity. Samples prepared with 25 % and 50 % of $P_{\text{N}_2}/P_{\text{total}}$ show reduced and nearly identical pre-peak amplitude, in agreement with their enhanced and similar resistivity values. By contrast, the samples prepared with 75 % and 50 % of $P_{\text{N}_2}/P_{\text{total}}$ show an increased pre-peak intensity, what can be related to their smaller electric resistivity, decreasing the electrical resistivity as the pre-peak intensity increases.

Sample prepared with 0% of N_2 , on the other hand, exhibits different XAS features. However, its pre-peak intensity follows the same evolution as the electric resistivity, laying between samples with 75 % and 50 %.

Fig 1(b) exhibits the differences between $[\text{MnN}_{x(1.5 \text{ nm})}/\text{Si}_3\text{N}_{4(3\text{nm})}]_{10}$ samples with $P_{\text{N}_2}/P_{\text{total}}$ ratio of 25% and 100 %.