Experiment MA-1405 report

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Experiment

The name of the experiment MA-1405 which took place in BM25A from 28/9/2011 to 2/10/2011 was: "EXAFS Characterization of ZnO/porous silicon/Si interfaces prepared by the Sol-Gel technique".

Samples

The samples studied were composed by zinc oxide (ZnO) grown on porous silicon substrates (PSi). 22 samples (of a total of 22) were succesfully measured.

Measurements

The principal objective of the measurements was to study the atomic neighbouring of Zn atoms, especially the oxigen (O) vacancies. The technique used was X-ray absorption fine structure (XAFS) in fluorescence mode. Samples were very thick, making the transmission mode unsuitable to measure. Zn atoms were used as absorbers, so the working x-rays energy was set at $9659keV$. Only the Zn metallic layer used as reference was measured by transmission.

Results and conclusions

One very relevant property of this material for applications in optoelectronics is the green photoluminescence at room temperature. Most publications assign this effect to O vacancies, but the experimental approaches are not conclusive. Another explanation attributes the luminescence to Zn vacancies, which is empirically supported and has a theoretical basement.

We have studied the photoluminescence of ZnO deposited on porous silicon (PSi) substrates. The ZnO/PSi structures were grown by the sol-gel method. Wurzite-type ZnO crystallites are obtained after sintering at temperatures over 200°C. In order to optimize the ZnO/PSi system, the samples were annealed at different temperatures and coated with different numbers of layers.

X-ray absorption fine structure (EXAFS) helped to determine accurately the local atomic distribution demonstrating an important Zn deficiency as

seen on Fig. (1) (upper left). Zn atoms are the principal contribution to the peak centred at 3Å, and that peak is smaller for higher annealing temperatures. On Fig. (1) (upper right) there is a temperature were the relation between the relative height of the Zn peak and the O peak centred at 1.5Å, is higher for the samples annealed at higher temperatures. This is related with the formation of ZnO because for annealing temperatures below 400°C the crystallites are very small and the effects of fluorescence are not visible. This is supported by Fig. (1) (lower left), were a quadratic-like behaviour shows a higher Zn signal when more layers are deposited. Fig. (1) (lower right) is a 2D map showing the relation between the annealing temperature and the number of layers deposited on each sample. The number of deposited layers is also important, because the more deposited layers, the bigger ZnO crystals and the effect becomes more visible as well as the higher the temperature, the higher the relation between the height of Zn and O although it seem to have a maximum around 600°C. On Fig. (2), images taken on a fluorescence microscope when UV light is exciting electrons from the valence band to the conduction band show a clear difference between the sample annealed at 600°C and the other one annealed at 800°C. The green emission is stronger for the sample annealed at higher temperature. This fluorescence can be explained by the formation of Zn vacancies due to the high temperatures and contributes to determine its origin.

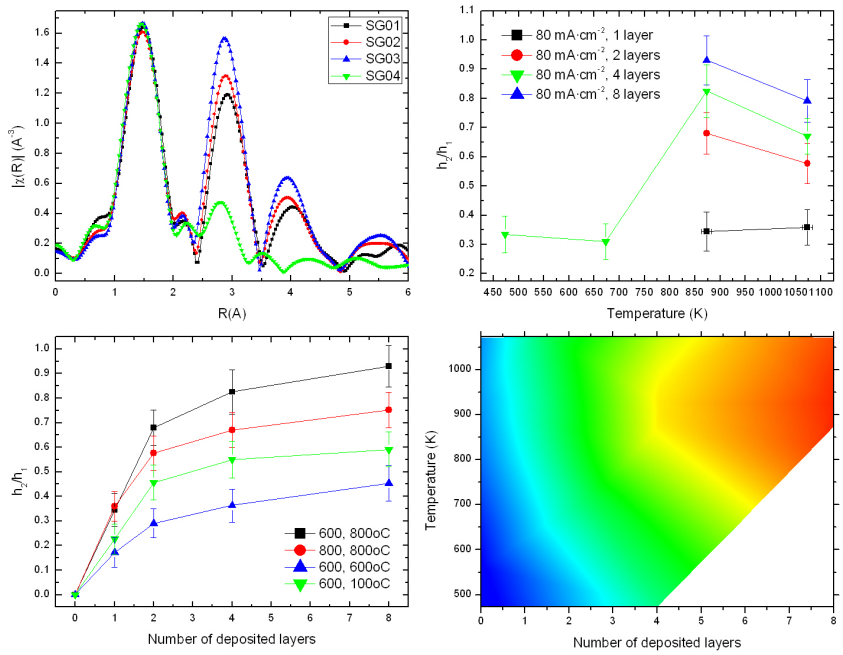
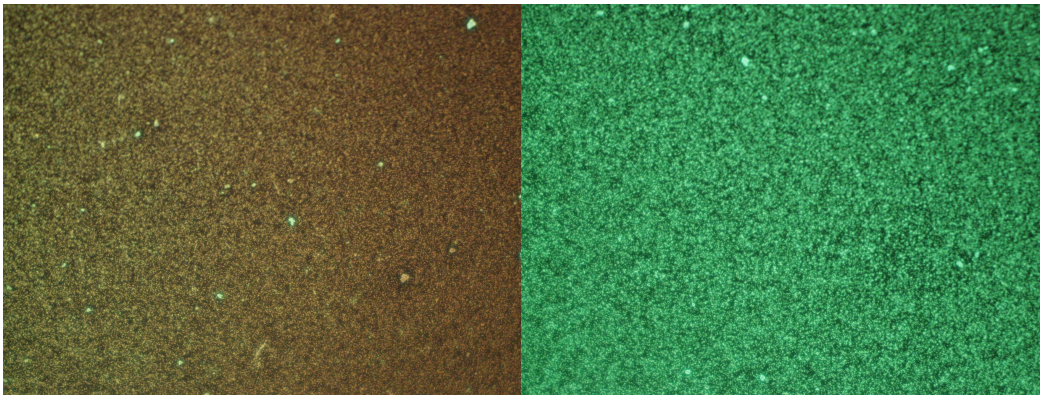


Figure 1: *Upper left:* Fourier transformed data for the samples annealed at 200°C, 400°C, 600°C and 800°C. *Upper right:* Relative height of the second peak (corresponding principally to Zn atoms and) and the first peak (corresponding to O atoms) for samples with different number of deposited layers as a function of annealing temperature. *Lower left:* Relative height of the Zn/O peaks nearest neighbours for samples annealed at different temperatures as a function of deposited layers. *Lower right:* Contour map of the Zn/O peaks relative height as a function of temperature and number of layers



(a) 600°C (b) 800°C

Figure 2: Fluorescence of the samples annealed at (a) 600°C and (b) 800°C while they were excited with UV light.