Scanning Photoelectron Microscopy (SPEM) of N-doped ZnO films: impact of carbon on the electronic band structure at the nanometer scale

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The *p*-type conductivity of ZnO has been the subject of extensive research for over 20 years. Although the problem has not yet been solved, systematic studies combining modern research techniques supported by advanced theoretical calculations and tailored growth technology provide interesting new results. Recently, it was found that the macroscopically measured *p*-type conductivity of ZnO may have a complicated microscopic origin, as shown by recent low temperature cathodoluminesence (LTCL) and scanning photoelectron spectroscopy (SPEM) studies that revealed separated donor and acceptor regions in ZnO:N.[1-2] A Scanning Photoelectron Microscopy (SPEM) experiment reported here was performed on the ZnO:N film deposited by Atomic Layer Deposition (ALD) under O-rich conditions, both *as grown* and post-growth annealed in oxygen at 800ºC.

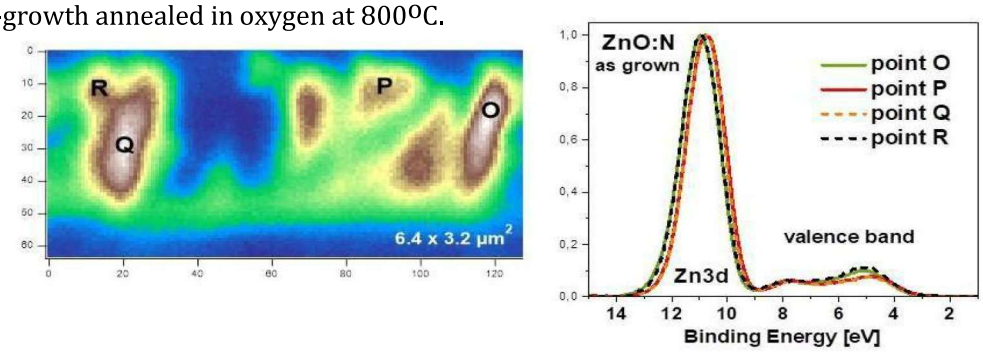

Figure 1. (left) SPEM image of the cross-section of the *as grown* ZnO:N film showing the points where PES spectra were taken; (right) PES spectra of the Zn3d and the valence band region taken at points O, P, Q and R.

Photoelectron spectra of *as grown* and annealed ZnO:N/Si films taken with *State-of-the-Art* resolution of 130 nm show significantly different intensities of the valence maximum close to the VB edge depending on the measured point of the film cross-section as well as a shift of some of the spectra towards the bandgap, pointing to hybridization with shallow acceptor states. We have found a significant correlation between a valence band shift and carbon content established from the intensity of the C1s state. The calculated migration properties show that complexes such as $V_{Zn}(NH)_O$, that are the source of acceptor states, are easily formed in the presence of the interstitial C_iH_2 group.[3] The presence of CH_2 groups in the samples leads to lowering of the migration energy by 0.8 eV and to zero in the ZnO and N:ZnO, respectively. These results confirm that the formation of defect complexes is very sensitive to the local geometry and lattice perturbations.

Acknowledgements: This project was financed by the NCN Project No. 2018/31/B/ST3/03576.

References

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