Study of the physical mechanisms leading to compositional biases in atom probe tomography of semiconductors.

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Laser-assisted Atom Probe Tomography (La-APT) is a powerful tool for investigating the 3D atom distribution in a wide variety of semiconductor materials. However, important compositional biases affect atom probe analyses. In the thesis, a systematic study of selected binary (GaN, GaAs, ZnO) and ternary (AlGaN, MgZnO) semiconductors was developed in order to identify the physical mechanisms leading to these biases. The results obtained highlight the effect of preferential evaporation of metallic species (Ga, Al, Zn, Mg) at high field conditions. Moreover, the emission of neutrals (N_2, O_2) at low field was proposed.

Another important aim of this thesis is to study both composition and morphology of some devices of technological interest, such as multi-Quantum Well (QW) systems. In this perspective, the knowledge of both 3D composition and morphology is essential because these features determine the optical properties of the systems. In order to do it, a correlative microscopy approach can be adopted. This approach was successfully applied to the study ZnO/MgZnO multi-QWs designed for quantum cascade lasers. Structural, compositional and optical properties were investigated performing correlative La-APT - Electron Tomography (ET) - micro-PhotoLuminescence (µ-PL) on atom probe specimens. The complementary La-APT and ET analyses reveal important decomposition phenomena in MgZnO alloys (fig. a, b). In particular, La-APT is proved to be a unique technique for a direct assessment of local composition. Moreover, µ-PL provide important information related the MgZnO composition, supporting La-APT results (fig. c).

Finally, a new correlative in-situ approach in which La-APT and µ-PL are simultaneously performed is presented. The development of a specially designed tomographic atom probe allows performing µ-PL on a single Zno/MgZnO atom probe tip during La-APT. This new approach is extremely attractive and challenging because allows to strictly correlating the variation photoluminescence signal with nano-metric scale volumes of the specimen evaporated during La-APT. In principle, the emission of single quantum light emitters (i.e. single QW) can be revealed. The new approach presented can be extended to a wide range of materials, opening new perspectives for correlative studies of single atom probe tips.

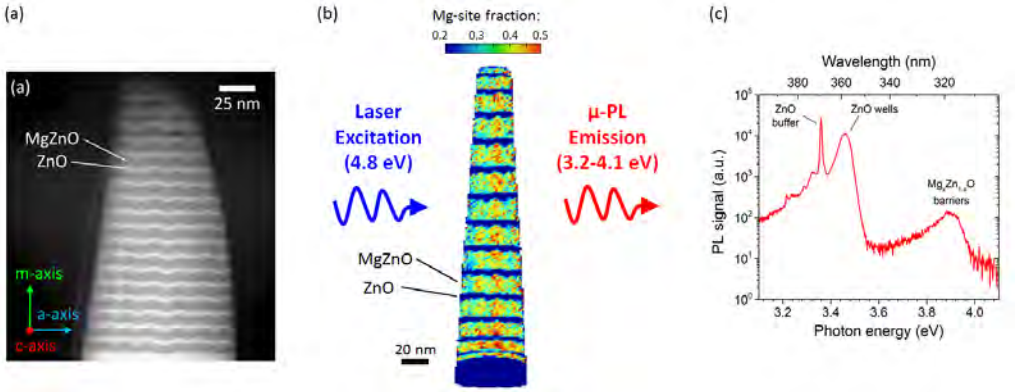

Figure: (a) STEM-HAADF image of ZnO/MgZnO multi-QWs. **(b)** Mg-site fraction map calculated from an atom probe tomographic 3D reconstruction. **(c)** µ-PL signal of a ZnO/MgZnO multi-QWs system acquired from an atom probe tip.