Three-dimensional atomic-scale investigation of ZnO-$Mg_xZn_{1-x}O$ m-plane heterostructures

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Abstract:

Heterostructures based on ZnO/$Mg_xZn_{1-x}O$ multi quantum wells (MQWs) are currently being considered for the development of devices based on quantum confinement effects and on interband or intersubbad transitions [1,2,3]. Quantum confinement effects in ZnO nanostructures are observed if the size of the structures is in the order of few nanometers: in ZnO/$Mg_xZn_{1-x}O$ MQWs structures, the ZnO layer thickness ranges typically from ~1 nm to ~4 nm obtaining materials with bandgap between ~3.8 and ~3.4 eV [1,4,5]. In this perspective, the knowledge of both composition and morphology of the heterostructure is essential because these features determine the optical and electrical properties of the system.

In this presentation a ZnO/$Mg_xZn_{1-x}O$ MQWs system has been studied adopting a correlative microscopy approach. Structural, compositional and optical properties have been investigated performing correlative Atom Probe Tomography (APT) - Electron Tomography (ET) - micro-PhotoLuminescence (µ-PL) on atom probe tip specimens. The complementary APT and ET structural analyses yield a clear picture of both morphology and composition of the MQW system. In particular, APT allowed a direct assessment of the alloy composition. These structural data has been compared with the optical properties of the system, measured by µ-PL on atom probe tip specimens. Finally, effective mass calculations were performed in order to correlate the structural data obtained by ET and APT with the optical properties of the system.

The ZnO/$Mg_xZn_{1-x}O$ MQWs system investigated in this contribution were prepared on a ZnO buffer that exhibits an unusual V-groove grating profile along the a-axis. The same geometry is adopted by all the layers growth on this ZnO buffer. In this configuration, the presence of vertical Zn enriched regions in $Mg_xZn_{1-x}O$ layers is suggested by HAADF-STEM contrast (fig. a) and confirmed by APT (fig. b). Such features appear in correspondence of the V-groove grating bottom edges. Simulations shows that the irregular profile of the QW layers and the compositional inhomogeneity of the $Mg_xZn_{1-x}O$ barriers yield carrier localization at the bottom groove edges, especially for holes (fig. c), with the consequent transition from a 2D confinement typical of a quantum well to the 1D confinement typical of a quantum wire. The optical properties of the system, including the possibility of measuring a PL signal from FIB-milled atom probe tip specimens, are in agreement with this localization mechanism.

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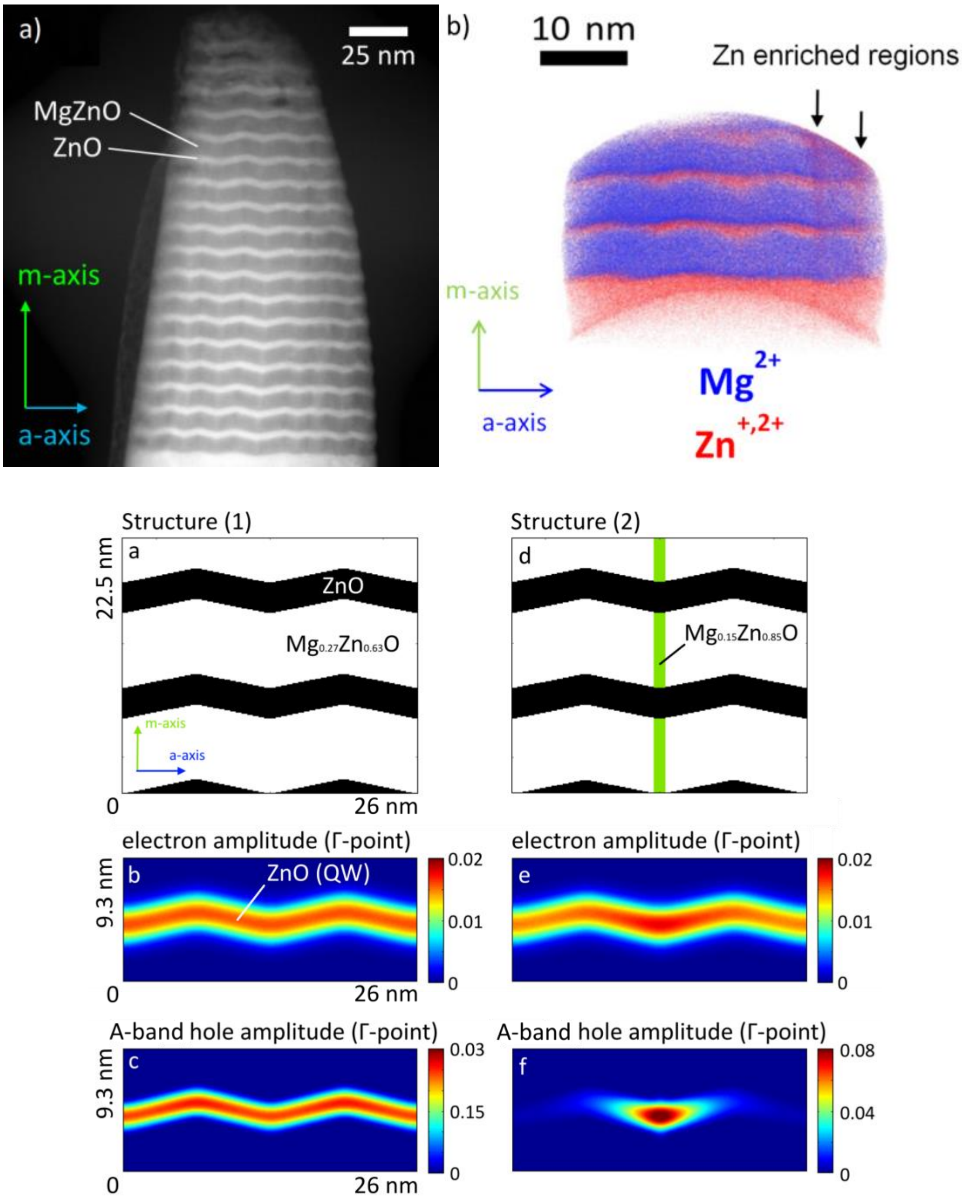

Figure: (a) STEM HAADF image of a ZnO/$Mg_xZn_{1-x}O$ atom probe specimen. The white layers are the ZnO QWs, the darker ones are the $Mg_xZn_{1-x}O$ barriers. **(b)** Atom probe tomographic reconstruction of the position of $Zn^{+,2+}$ (red) and Mg^{2+} (blue) atoms. **(c)** The V-groove grating structure (1) and the amplitude of the electron (2) and A-band hole (3) wave-function associated to the ground state at the Γ-point for a ZnO QW. The effect of a vertical Zn-enriched region (4) on the quantum confinement is reported for electrons (5) and A-band holes (6).