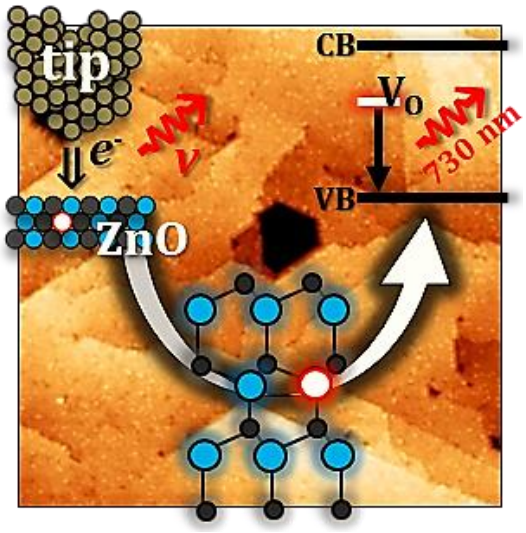
STM Luminescence Spectroscopy of intrinsic defects in ZnO (0001) thin films

Fernando Stavale[1,2,*], Leandro Pascua[1], Niklas Nilius[1,3], and Hans-Joachim Freund[1]

[1] Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany
[2] Centro Brasileiro de Pesquisas Físicas, R. Dr. Xavier Sigaud 150, Urca-22290-180 Rio de Janeiro, Brazil
[3] Carl von Ossietzky Universität Oldenburg, Institut für Physik, D-26111 Oldenburg, Germany

*stavale@cbpf.br



Over the last hundred years, zinc oxide has been widely applied as white pigment, antiseptic substance, as transparent oxide for solar cells and gas sensing. Although, enormous progress on the use of ZnO has been made over the years [1], some key fundamental questions are still not well understood regarding the role of its intrinsic defects on the electric and optical properties. Previous studies have suggested that defects are responsible for the widely observed n-type conductivity of the material, although it was accepted only recently that lattice-hydrogen serves as the hidden donor. At present, insights into the nature of native ZnO defects comes mostly from theoretical studies [2], while experimental results are not always conclusive and sometimes in conflict to each other [3]. In this study, we have prepared well-defined ZnO films on Au(111) substrate as a model-system and investigated the luminescence response locally by scanning tunneling microscopy and cathodoluminescence spectroscopy. In order to relate the observed emission peaks to intrinsic defects, we have varied the ZnO growth conditions, e.g. the temperature and O2 pressure, and reduced the films with atomic hydrogen and laser irradiation. In well-prepared films, band recombination gives rise to the dominant peak at 373 nm, while three additional peaks at higher wavelength indicate the presence of defects in the oxide lattice. To identify the nature of these emission centers, the abundance of typical ZnO defects has been varied by purpose. Film growth at reducing conditions produces a prominent band at 730 nm, suggesting a correlation to O-vacancies in the lattice. Incorporation of atomic oxygen, on the other hand, leads to an increase of the 595 nm emission peak. Varying the availability of Zn during film growth finally modulates the intensity of the 535 nm defect line. The results of our luminescence data are summarized in an energy diagram of the ZnO defect levels and compared to recent DFT calculations. Our study [4] offers conclusive evidence on the nature of the underlying lattice defects, providing a correlation between structural, electronic and optical properties of ZnO.

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