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Intrinsic and Extrinsic Defect Structures in Zinc Oxide (ZnO) Nanoparticles

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Extended Abstract

Comprehensive understanding of the defect centers in zinc oxide (ZnO) nanoparticles invokes an important issue of controlling the nanoscopic properties of ZnO compounds. Due to its wide band gap (3.4 eV), ZnO possesses extraordinary electronic and optical properties, which make it a very attractive material for technological applications, such as thin film printable electronics. Doping ZnO with transition metal ions, like Fe, Co, or Mn leads to materials with diversified behavior towards magnetic and optical excitation. Even relatively small concentrations of defects and impurities can significantly affect the electronic, magnetic and optical properties of semiconductors. Therefore, understanding the role of defect centers (i.e. vacancies, interstitials, and antisites) and the incorporation of stable or meta-stable defects is a key tool toward controlling the electronic properties of ZnO. EPR is well suited for this task since it provides a direct method to monitor different paramagnetic states of vacancies and, thus, complements other experimental techniques such as photoluminescence. In this sense, EPR does not only work very well on the identification of defects but also one may obtain reliable correlation to the luminescence properties of bound excitons. Nonetheless, just from the basic principles of defect formation, it is hard to understand or predict what kind of defects will be present in the sample. From the EPR point of view, so far different EPR spectra have been assigned to the same defect site, or the same spectrum has been assigned to the different paramagnetic centers in ZnO. Thus, the nature of the defects and the interpretation of the defects are still controversial issues. In this work, undoped ZnO nanoparticles were synthesized by decomposition of zinc oximate [1] and the doped samples were synthesized by coprecipitation method. In order to characterize the ZnO defect structure, both light induced X band and high field EPR has been applied. To understand the behavior of defects in ZnO nano-particles under light, we imposed *in-situ* laser light with wavelengths of 445 nm (2.78 eV) and 532 nm (2.33 eV) on the samples during the X band EPR measurements. This is crucially important since defect structures may show different properties under different wavelength. Ultra-high frequency EPR measurements over the temperature range 2-300 K were performed on the 15/17 T transmission instrument. EPR measurement at 208 GHz allowed to resolve small differences in the *g*-values. The two different *g*-factors of 2.0028 and 2.0000 originated from different defect centers located at the *surface*. Moreover, the 406 GHz EPR result showed that the signal from the *surface* was due to three different paramagnetic defect centers.