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# Optoelectronic Properties of Hexagonal Wurtzite Yb-doped ZnO using VEELS

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ZnO nanoparticles have been attracting the attention of the scientific community due to exhibiting wide range of applications which covers nano optoelectronic devices, sensors and transducers. ZnO possesses a thermodynamically stable wurtzite structure with hexagonal phase and P63mc space group. This material is considered as an n-type semiconductor with a direct bandgap of $E_g$ = 3.37 eV at room temperature [1]. In order to improve other potential applications with thermoluminescence properties, few reports monitored the effect of $Yb^{3+}$ as a dopant in the ZnO nanoparticles [2]. The motivation of this work is to determine the electronic and optical properties of polycrystalline wurtzite Yb-doped ZnO (ZnO:Yb) through electron energy loss spectroscopy in the valence region (VEELS). The Kramers-Kronig analysis (K-KA) using the Gatan microscopy suite routines have been performed to obtain the electron energy loss function (ELF), complex dielectric function (CDF) and the optical absorption coefficient, μ for ZnO:Yb.

The polycrystalline ZnO:Yb nanoparticles were prepared by the glycol mediated chemical synthesis. For Yb doping, 1 and 5 mol% was added to the reaction mixture before the heat treatment [2]. Previous to acquiring the EELS for this material; Rietveld refinement x-ray diffraction (XRD) analysis (using Fullprof software [3]) confirmed the hexagonal wurtzite structure considering the P63mc space group. The EEL spectra were acquired by an EELS GAT-777 STEMPack attached to a JEM-2200FS microscope working at 200 kV in the TEM mode. To analyze the acquired low loss EELS spectrum, we take into account the deconvolution of the zero-loss peak (ZLP). The Fourier-log method to remove plural scattering and K-KA was carried out using the Gatan microscopy suite software.

Figure 1(a) shows the bright field (BF) electron micrograph to monitored the ZnO:Yb(5%) morphology with quasi-rounded faceted nanoparticles. Panel (b) displays the histogram (Image J software) to determine the particle size distribution of about 96 particles with the corresponding log-normal fit using the Levenberg-Marquardt iteration process (OriginPro software). The selected area electron diffraction pattern (SAED) and comparison to a simulated set of continuous ring patterns using crystallographic toolbox (ring GUI) software [4]. We considered for SAED ring diffraction analysis, the CIF file from XRD analysis. Figure 2(a) shows the low-loss EELS region, identifying the three principal components. The pronounced peak at 0 eV is labeled as the zero-loss peak (ZLP). The energy range of ~10-30 eV is dominated by the plasmon peaks. [3] In this panel, ELF is also displayed. Panel (b) reveals the K-K relations relating the real and imaginary parts of the CDF, $\varepsilon^* = \varepsilon_1 + i\,\varepsilon_2$ [4]. The variation of μ (panel c) and the direct $E_g$ = 3.4 eV was determined according to the method proposed by Rafferty and Brown [5].

This result corroborates that the prospective ZnO:Yb(5%) has potential applications in optoelectronic devices [6].

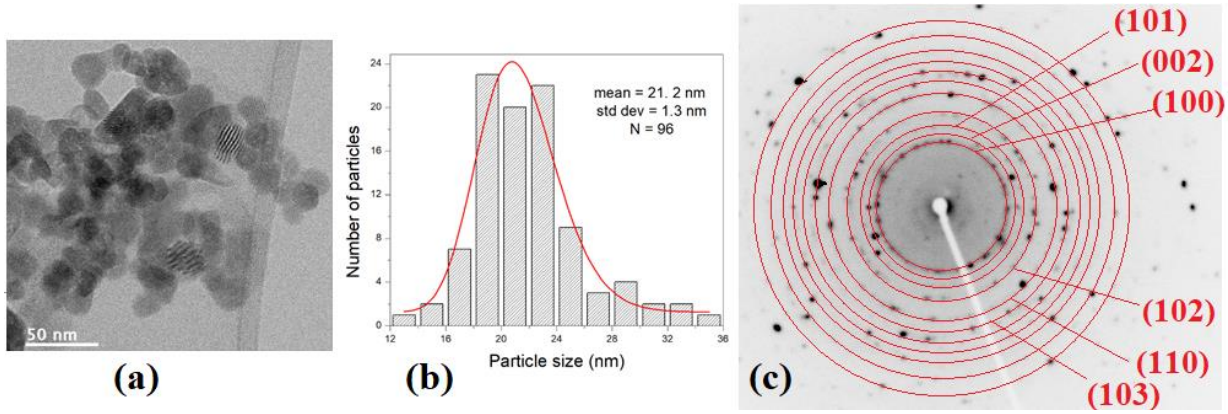


**Figure 1.** (a) BF electron micrograph showing quasi-rounded nanoparticles. (b) The size distribution histogram and corresponding log-normal fit. (c) SAED pattern for ZnO:Yb(5%).

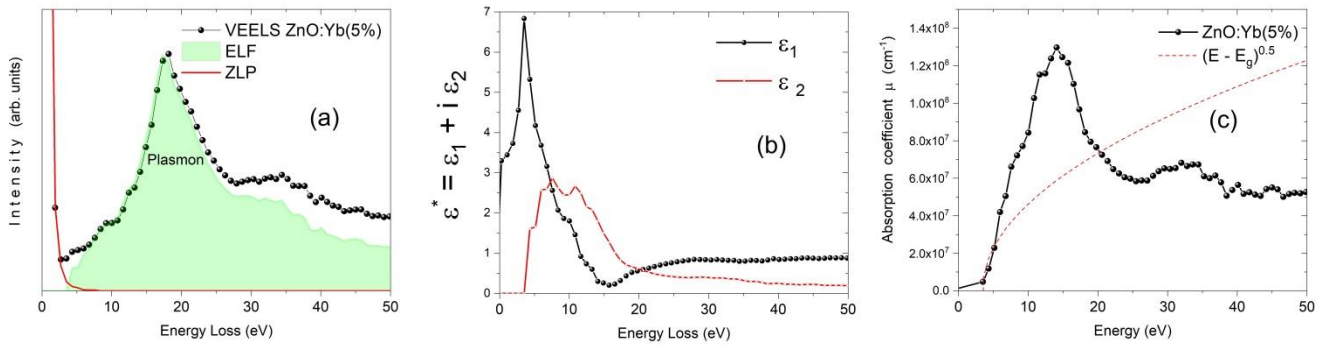


**Figure 2.** (a) VEELS region, ZLP deconvolution and ELF (green filled area under the curve). (b) Real and imaginary parts of the CDF. (c) The variation of μ and direct $E_g$ determination using a polynomial fit.

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