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Structural characterization and EXAFS wavelet analysis of Yb doped ZnO

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Lanthanide doped Zinc oxide (ZnO) are interesting materials for both optical[1] and electrical[2] applications. The wide band gap of this semiconductor makes it transparent in the visible range (Egap = 3.2 eV), allowing a sharp emission (<1nm) from the lanthanides intra shell transition due to the low influence of the crystal field.
From the electrical side, ZnO is a widely used material in varistors and its electrical properties can be tailored by the judicious inclusion of lanthanides. Both applications are influenced by their location: grain boundaries segregation, lattice inclusion, substitution, etc.[3-4] Yb doped ZnO samples obtained by a wet chemistry route were annealed at different temperatures and characterized by Transmission Electron Microscopy (TEM), X-ray Diffraction (XRD), Rietveld refinement, and X-ray Absorption Fine Structure (XAFS). These techniques allowed to follow both the changes occurred in the matrix and the Yb environment. The use of the Cauchy continuous wavelet transform allowed identifying a second coordination shell composed of Zn atoms, supporting the observations from Rietveld refinement and XAFS fittings. The analysis confirmed the incorporation of Yb in Oh sites of the wurtzite structure without Yb_2O_3 clustering in the lattice.

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