Revealing the effect of Tb doping in ZnO nanoparticles by studying its structural and magnetic properties

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Abstract

Introducing rare earth ions in the host semiconductor oxide crystal at nanoscale affects the luminescence as well as the structural properties of semiconductor host crystal due to the interaction between these dopant ions and host crystal. We have synthesized Tb doped ZnO nanoparticles using sol gel method. A systematic structural studies on Tb3+ ion doped ZnO nanoparticles were carried out using X-ray diffraction, X-ray photoelectron spectroscopy and photoluminescence studies. These experiments were performed to study the defects induced in the ZnO host lattice when rare earth ion of ionic radii more than that of Zn ion is doped in the ZnO nanoparticles. Elemental compositions of the pure and doped samples were identified by EDX measurement. The dislocation densities and the surface area calculation from the XRD profile show an increase up to a certain concentration of Tb, which reveals the increase in the surface defects when Tb is incorporated in ZnO host lattice. The strain calculated using Uniform deformation model UDM from the XRD data also show an increase in the stress with the increase in Tb doping concentration which reveals the deformation of the host lattice. The order of distortion (R as calculated using XRD data) is also observed to follow the same trend. It has been observed that the value of u (positional parameter) decreases slightly in such a way that the four tetrahedral distances almost remain nearly constant by distorting tetrahedral angles. The Zn–O bond length calculated for our nanoparticle samples comes in the range of 1.9669 Å–1.9812 Å. There is a good agreement of the calculated & actual bond length which supports the results of present study. The PL studies performed on these nanoparticle samples show the presence of band edge emission as well as emission due to complex defects. Room temperature magnetic properties have been measured using VSM and revealed the coexistence of paramagnetic and weak ferromagnetic ordering in Tb3+ doped ZnO nanoparticles.A slight shift in reflection peaks of the diffraction pattern of Tb substituted ZnO nanoparticles to higher angle than those of pure zinc oxide nanoparticles is observed. It shows that incorporation of Tb3+ into ZnO nanoparticles creates some defects which modify the ZnO crystal. However, an insight analysis of the position of the XRD peaks indicates shifting of peaks towards lower angle with further rise in Tb ion content. The change in the position of peaks (1 0 0) (0 0 2) and (1 0 1) clearly shows that Tb ion is modifying the surface either by accumulating on the ZnO nanoparticle to some extent and also getting incorporated for higher Tb mole fraction. The primary investigation doesn't show the traces of Li in the nanoparticle samples. A slight shift in peak positions, and their full width at half maximum (FWHM) in the samples having different Tb content as compared to the undopedZnO nanoparticles has also been observed. This shift could be attributed to the strain generated on the host lattice and replacement of some zinc ions with that of Tb3+ ions. It has been reported in the literature that with addition of foreign particle/dopant in the crystal lattice, a strain and defect(s) is introduced in the lattice which may result in reduction of crystal quality. The peak broadening of the XRD profiles clearly indicates that nanoparticles are present in the samples. There is no evidence of impurity phase in the XRD profiles.

The dislocation density and the specific surface area of the prepared samples are also estimated using the XRD data. The obtained values of specific surface area shows an increase with Terbium concentration which clearly suggests that in a given regime the Tb is mostly present on the surface as defects. But at a later stage when Tb is incorporated further, the value of surface area goes down as the Tb now gets incorporated in the ZnO lattice. The value of dislocation densities and specific surface area clearly indicates that the ZnO host lattice gets modified with the incorporation of Tb in it. Surface energy density γ has to be positive in order to have a compressive hydrostatic strain in the lattice. γvalue were also estimated using the a and the c lattice constants. The values of γ as a function of the Tb mole-fraction clearly show an increase with x, which is due to the increase of the Tb coverage on the surface of the nanoparticles with the increase of Tb mole-fraction. This surface induced hydrostatic strain is also responsible for the enhancement of the band gap energy with the Tb mole-fraction. The strain for all the nanoparticles was estimated which reveals that the value of strain increases with the increase in Tb concentration up to x = 0.04 while it decreases further for Tb concentration beyond x = 0.04. This observation is in agreement with the results obtained from the XRD data.