



Influence of pH and Fe doping on structural and physical properties of $\text{Mg}_{0.95}\text{Mn}_{0.05-x}\text{Fe}_x\text{O}$ ($x = 0, 0.04$) nanoparticles

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ABSTRACT

We investigate the effects of pH and Fe doping on the size, structural and physical properties of $\text{Mg}_{0.95}\text{Mn}_{0.05-x}\text{Fe}_x\text{O}$ ($x = 0, 0.04$) nanoparticles. All the nanoparticles were synthesized by the sol-gel autocombustion method by varying the pH of the solution. Furthermore, the phase purity, size, and size distribution of the nanoparticles were studied by powder X-ray diffraction (XRD), scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Irrespective of the pH, Rietveld refinement analysis of the XRD data reveals single crystallographic cubic phases with MgO-type wurtzite structure (space group $Fm\bar{3}m$) along with a lattice parameter of 4.2121(8) Å for $x = 0.0$ and 4.2083(5) Å for $x = 0.04$. This change in lattice parameter with Fe doping is due to the smaller size of Fe^{2+} (78 p.m.) compared with Mn^{2+} (83 p.m.). The size of the nanoparticles increases monotonically from approximately 10 nm to approximately 16 nm for $x = 0.0$ and from approximately 18 nm to approximately 23 nm for $x = 0.04$ with increasing pH. SEM micrographs of the powders show highly agglomerated nanoparticles with porous and irregular morphology. The TEM findings support the XRD results, showing that the nanoparticles increase in size with increase in pH. Because Raman modes should be absent in bulk MgO and present in MgO nanoparticles, the strong intensity of the three Raman modes at approximately 380 cm^{-1} , 470 cm^{-1} , and 608 cm^{-1} further supports the formation of small nanoparticles of $\text{Mg}_{0.95}\text{Mn}_{0.05-x}\text{Fe}_x\text{O}$ ($x = 0, 0.04$). The decrease in peak intensity with increase in pH suggests an increase in the size of the nanoparticles. The peak at 470 cm^{-1} corresponds to a transverse optical phonon, while the peak at 380 cm^{-1} corresponds to a transverse acoustic phonon.

1. Introduction

The synthesis of nanocrystalline semiconductor oxide materials have recently attracted considerable interest because of their unique physical and chemical properties leading to multifunctional applications, such as catalysis, sensing, electronics, and energy storage [1–5]. The alteration of these semiconductor oxides by different dopant elements led to a scientific breakthrough that helps to meet the demands of advancing technology depending on the desired electronic, optical, and chemical applications of these materials [6]. The search for spintronic materials that combine both semiconducting and ferromagnetic properties is currently one of the most active research fields. In this direction, much research work has been done on the introduction of transition metal and rare earth atoms into semiconducting materials

because they can introduce favorable magnetic properties in a controllable fashion [7]. These magnetic semiconducting materials with room-temperature ferromagnetism and controllable semiconducting properties are important for spin-polarized current generation in modern electronic device applications [8,9]. Most of the efforts in magnetic ion doping have been devoted to III-V semiconductors, with a few exceptional studies on II-VI semiconductors, especially on zinc oxide [10,11]. To explore this field of semiconductor oxides, work has been performed on dilute magnetic insulator or transition metal-doped insulator MgO-based microstructured/nanostructured metal oxides.

Bulk ZnO, MgO, and TiO_2 are among the most studied semiconductor oxides because of their electrical and optical properties. Particularly, focus on the optical and electrical properties of coupled semiconductors such as Mg_2TiO_4 has increased recently [12–15]. Bulk

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