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Systematic investigation of structural and morphological studies on doped TiO_2 nanoparticles for solar cell applications

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ABSTRACT

Optical, structural and thermal properties of the doped with different ions (transition metals, other metals or post transition metals, non-metals, alkali metals and lanthanides) in TiO_2 nanocrystals were investigated. The doped nanoparticles were synthesized by modified chemical method. Ethanol–deionised water mixer (20:1) was used as solvent for synthesize of the undoped and doped TiO_2 nanoparticles. Systematic studies on structural and morphological changes by thermal treatment on TiO_2 were examined. It has been observed that with Eu and Al doping TiO_2, the phase transition temperature for anatase to rutile phase increased. Blue and red shifting absorptions were observed for doped TiO_2 in visible region. Among the dopant, significant blue shift was obtained for Cu, Cd, Ag, Y, Ce and In doped TiO_2 and red shift was obtained for Zr, Sm, Al, Na, S, Fe, Ni, Eu and Gd doped TiO_2 nanoparticles.

1. Introduction

Titanium dioxide (TiO_2) is an important semiconductor nanomaterial for use in a wide range of applications such as photocatalysis, environmental pollution control separations, sensor devices,

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paints, and solar cells [1–4]. The material properties of TiO_2 nanoparticles are a function of the crystal structure, nanoparticle size and morphology and, hence, are strongly dependent on the method of synthesis [5–8]. It is well known that titanium dioxide exists in three crystalline polymorphs, namely rutile (tetragonal), anatase (tetragonal), and brookite (orthorhombic) [8]. Due to the enormous technological importance, TiO_2 nanoparticles have been under intensive investigation for the past years by both experiments and computer simulations. Control of the conditions that affect the kinetics to control the anatase to rutile phase transformation is of considerable interest. This is particularly the case for high-temperature processes and applications, such as gas sensors and porous gas separation membranes [9,10], where the phase transformation may occur, thereby altering the properties and performance of these devices.

To enhance the photocatalytic effect in the visible light region, many producing methods were proposed to dope (or incorporate) trace impurity in TiO_2 including: ion-sulfate process [11], chloride process [11], impregnation [12], co-precipitation [13], hydrothermal method [14], direct oxidation of $TiCl_4$ [15], assisted sputtering, plasma, ion-implantation [16], chemical vapour deposition [17] and sol–gel [18]. Among these methods, the sol–gel process is commonly used for synthesis of nanocrystalline TiO_2. This technique does not require complicated instruments and provides simple and easy means for preparing nano-size particles [19,20]. The incorporation of an active dopant in the sol during the gelation stage allows the doping elements to have a direct interaction with support, therefore, the material possesses catalytic or photocatalytic properties.

Metal ion doping was demonstrated to be able to modify the absorption spectrum of TiO_2 nanoparticles. Visible light photoactivity of metal-doped TiO_2 can be explained by a new energy level produced in the band gap of TiO_2 by the dispersion of metal nanoparticles in the TiO_2 matrix. There are three different main opinions regarding modification mechanism of TiO_2 doped with different ions: (i) band gap narrowing; (ii) impurity energy levels and (iii) oxygen vacancies. In this work, we focus on the investigation of effect of the selected transition metals, post transition metals, alkali metals, non metals and lanthanides doping on TiO_2 nanoparticles. The pH was exhibited about constant for all the colloidal solution. Crystalline nature and morphology of the corresponding samples were systematically investigated. Optical and thermal behaviour of the doped samples were studied.

2. Experimental method

2.1. Materials

All the chemicals were of analytical reagent grade and used without further purification. Titanium tetra-isopropoxide (TTIP, 97%, Aldrich) was used as the precursor for titanium dioxide synthesis. Dopant, europium (III) nitrate (99.9%) was purchased from Aldrich, copper (II) acetate (98%) and sodium sulfide flakes were obtained from Fisher scientific company, silver nitrate (99.8%) was obtained from Universal Laboratory, cadmium chloride (99%), zirconium oxychloride (99%) and nickle (II) chloride hydrate purified (97%) were purchased from Merk, iron (II) chloride tetrahydrate (99%), cerium (III) nitrate hexahydrate (99.5%), samarium (III) oxide (99.9%), aluminium chloride (99%), gadolinium (III) oxide (99.99%) and indium (III) acetate (99.9%) were purchased from Alfa Aesar, yatrium oxide (99.99%) and sodium chloride were obtained from spectrochem, ethanol (99.9%) and Acetone (99.9%) were purchased from Hayman Speciality products.

2.2. Synthesis of doped TiO_2

The doped TiO_2 nanoparticles were synthesized by drop wise addition of titanium tetra-isopropoxide (TTIP) into selected dopant precursor (1%) and Polyvinylpyrrolidone (PVP, MW:40,000) in ethanol–deionised water matrix (20:1). The reaction was performed with continuous stirring for 2 h at 80 °C. The resulting solution was allowed to rest and cool back to room temperature. The suspensions obtained were dried in an oven for 2 h at 120 °C. To investigate the thermal stability, the obtained powder samples were further annealed for 2 h in a box furnace temperature at 400 and 800 °C in an ambient