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Original Research Paper

Generation of uniform tetrapod-shaped zincoxide nanoparticles by gas-phase reaction with using flow restrictor

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ABSTRACT

Tetrapod-shaped ZnO particles are generated via gas-phase reaction of Zn vapor and oxygen in air, where they undergo homogeneous nucleation from supersaturated ZnO vapor and successive growth by surface reaction. It was found that a simple device for flow restrictor is effective in making ZnO particles of terapod-shape by leaving sufficient amounts of unreacted Zn vapor with the embryos of ZnO. In the absence of the flow restrictor, only spherical particles are formed because the oxidation reaction takes place immediately after mixing and unreacted Zn vapor does not remain for the subsequent crystal growth. The Zn vapor concentration distribution, oxygen concentration distribution, temperature, gas velocity and reaction rate in the reactor were analyzed by using a conventional computational fluid dynamic simulation package. The simulation revealed that the flow restrictor does not enhance mixing between Zn vapor and air but suppresses the mixing and reduces the residence time in the reactor so that sufficient amounts of unreacted Zn vapor remain downstream of the flow restrictor, allowing ZnO particles to grow in tetrapod-shape by abnormal crystal growth.

1. Introduction

Nanoparticles have attracted great attention because their size alters the physical and chemical properties. ZnO, *n*-type semiconductor, are of great interest because of intriguing properties including unique optical functions originating from the wide band gap of 3.37 eV and high excitation binding energy of 60 meV [1]. Much intensive research about its unique properties and versatile applications, such as transparent electronics [2], ultraviolet (UV) light emitters [3], piezoelectric devices [4], chemical sensors [5], cosmetic [6] and photocatalytic activities [7] have been reported. The size and shape varieties of nanostructured ZnO reported are nanowhisker [8], nanowire [9], nanorod [10], nanoshell [11], etc. These unique morphologies are brought by the formation process of initial nuclei and the growth process, i.e., nucleation and growth.

Many synthetic routes of ZnO nanoparticles were reported, e.g., chemical vapor deposition [12], aqueous solution deposition [13], sol–gel method [14], decomposition of zinc nitrate [15], carbon thermal method [16], catalyst-assisted vapor–liquid–solid (VLS) mechanism [17] and oxidation of Zn vapor [18]. Gas-phase oxidation is one of the potential means to produce ZnO nanoparticles with high purity with high production yield. A typical mass production process of ZnO is the French process, in which ZnO nanoparticles are formed from zinc metal through vaporization and oxidation in a combustion zone. This direct and simple method has the potential to generate uniformly sized nanoparticles [19]. In general, the gas-phase reaction is difficult to control the mixing of metal vapor and oxidant to obtain uniform concentration distribution for generating monodispersed nanoparticles. Without the control of mixing, ZnO monomers tend to condense on existing nuclei growing to large particles of several micrometers which do not exhibit specific nanoparticle characteristics.

In order to investigate the influence of local concentration and temperature on the formation of ZnO particles, computational fluid dynamics has been employed by several authors [20,21]. The combination of CFD simulation with experiments could give good insight for studying the synthesis and crystal growth processes of ZnO.

In the present work, ZnO nanoparticles were prepared via gas-phase reaction and the characterization of formed nanoparticles was carried out. The control of local concentration distribution of Zn vapor and oxygen is the key to synthesis ZnO nanoparticles with a given shape. Consequently a mixing device (flow restrictor) was introduced for controlling the mixing between Zn vapor and oxygen in the reactor. The final goal of this work is to control the morphology of ZnO nanoparticles via gas-phase reaction by controlling the local synthetic parameters, such as the evaporation

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