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Structural, morphological, optical and gas sensing properties of nanocrystalline ceria thin films

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Abstract

Ceria thin films are deposited with varying oxygen pressures (1- 225 m torr) and at an optimized substrate temperature of 1023K on quartz substrates by pulsed laser deposition technique. X-ray diffraction studies indicated that the prepared thin films are polycrystalline in nature. The prepared thin films contain nano crystals of size in the range of 20-31nm. Crystallite size, strain and dislocation densities of the ceria thin films have been calculated. To know the preferred orientation of the films texture coefficient has been calculated. The characteristic Raman peak appeared at 463 cm^{-1} is associated with F_{2g} active mode confirm the cubic fluorite structure of ceria. Surface morphology of the thin films carried out by atomic force microscopy. The optical properties of the thin films are investigated by using UV-Vis spectroscopy technique in the wavelength range 200-800nm.The optical band gap, refractive index and absorption coefficient are calculated. Gas sensing characterization of ceria thin films have been carried out by chemiresistive method for various concentrations of acetone vapour and operating temperatures.

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Keywords: Ceria, thin films, XRD, Pulsed laser deposition, Raman spectroscopy, optical properties, gas sensing

1.Introduction

The sensors to detect volatile organic compounds have been attracted great attention due to their practical applications in protection of environment and safety. Among volatile organic compounds, acetone is the important organic compound widely used in laboratories and medical fields. It is a colorless, flammable liquid and the simplest ketone with chemical formula CH_3COCH_3 . The large quantities of acetone is emitted into the atmosphere by human body, plants, trees, volcanic gases, forest fires, as a product of the breakdown of body fat and industries. Acetone in environment can irritate, cause permanent eye damage and its long-time exposure can cause kidney, liver and depress central nervous system. Due to its complex nature, much attention has been given by the researchers to

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design and develop sensors with desired figure of merits for the detection of acetone. L.K.Bagal et al[1] reported gas sensing characterization of SnO_2 based materials towards acetone gas at high concentration of acetone. P.P.Sahay [2] investigated sensitivity of ZnO towards acetone vapour at high operating temperatures.

Rare earth oxides have been generated a lot of interest due to electronic and various optical applications such as optical filters, capacitors and sensors etc. Among these oxides, ceria is an ionic and insulating oxide with the fluorite structure. Ceria thin films have been attracting great interest due to its outstanding properties such as large band gap, high dielectric constant, high temperature and chemical stability, large refractive index and high transparency in the visible and near infrared regions. These properties uplift the use of cerium oxide thin films for potential applications such as stable capacitor with small size[3], electronic devices such as dynamic random access memory[4-5], radiation emitters for thermophotovoltaic systems[6], high temperature super conductor films, silicon-on-insulator structure[7]. High refractive index, absorption of ultraviolet radiation, transparency in the visible and near infrared region which makes cerium oxide thin films as an ideal UV blocker and appropriate replacement for titanium oxide and zinc oxide [8]. Ceria thin films have potential applications as single layer and multilayer optical coatings[9], electrical gate insulator material for metal –oxide-semiconductor transistor [10], electro-chromic windows [11], Photo catalysis and fuel cells [12]. In the present decade, ceria thin films have been applied for the detection of carbon mono-oxide, hydrogen, nitrogen oxide and acetone as resistive gas sensors [13-14]. Contemporary studies have shown that nanocrystalline thin films with good stoichiometry can be obtained by using pulsed laser deposition technique. Although lot of research work has done for cerium oxide thin films by using sol-gel method[15], R.F.Sputtering[16], spray pyrolysis[17], Flash evaporation[18], thermal evaporation[19], Reactive ion beam sputtering[20], laser ablation[21], electron beam evaporation[22], atomic layer deposition[23] and pulsed laser deposition[24-25]. Among all these methods, pulsed laser deposition is a simple and unique technique to deposit high quality thin films from a wide variety of compounds and materials. The main advantage of pulsed laser deposition is generation of hyper thermal species with huge kinetic energy in the order of 100eV. Deposition of hyper thermal species can increase the adatom mobility and hence, the film quality. There are several parameters included in pulsed laser deposition such as laser wavelength, oxygen partial pressure, substrate temperature, pulse repetition rate, source to target distance and laser energy that need to be optimized to obtain for gas sensor application. To the best of our knowledge, very little amount of work have been reported on ceria thin film as acetone gas sensor. The present investigation deals with the on the Structural, morphological, optical and gas sensing properties of nanocrystalline ceria thin films.

1. Experimental procedure

Commercially accessible ceria (99.99% purity) powder is compacted into pellet of 20mm diameter and 5mm thickness at a pressure of $3tonn/cm^2$ by using hydraulic pelletizer. The prepared pellet is sintered at 1673K for 8hours. The sintered pellet is used as a target material for pulsed laser deposition. Prior to the deposition the chamber is evacuated to 4×10^{-6} torr using turbo molecular pump backed with rotary pump. The quartz substrate is cleaned in an ultrasonic bath with acetone for 15 minutes and then washed with distilled water and dried in oven to make moisture free substrate. Deposition of ceria thin films on clean quartz substrates have carried out as a function of oxygen partial pressure(1 m torr – 225 m torr) at an optimized substrate temperature of 1023K, using KrF excimer laser(248nm) with laser energy density 2.5J/ , pulse repetition rate 10Hz, target to substrate distance 4cm and deposition time is 30minutes. The thicknesses of the thin films are measured by using XP-1 stylus profiler. The structural properties of thin films are studied by using high resolution X-ray diffraction system using a LiF monochromator with 15.4nm wavelength in the range of 20^o to 60^o with 1^o/min scanning speed. Surface morphology of the thin films has studied by atomic force microscope (AFM)(Digital instruments Inc, Nanoscope E, Model NSE,USA) with contact mode. The Raman spectra of ceria thin films is carried out in the back scattering geometry using an Argon laser excitation source emitting at 488 nm coupled to a Labram-HR800 micro-Raman Spectrometer at room temperature in the range of $100cm^{-1}$- $500cm^{-1}$ of Raman Shift. The optical transmittance of the prepared ceria thin films is measured at normal incidence mode at room temperature by using double beam UV-Vis spectrophotometer(Systrnics 2202, Ahmedabad, India) in the wavelength of 200-800nm with a spectral bandwidth of ~2nm in the transmittance mode).