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Detection and sensing mechanism of acetone with modeling using $Pd/TiO_2/Si$ structure

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ABSTRACT

A grided $Pd/TiO_2/Si$ (Pdtisin) gas sensor is fabricated to detect hydrocarbons such as acetone, ethanol and trichloroethylene. The sensitivity measurements are carried out in various ambient (O_2, N_2 and Ar) at room temperature which revealed that fabricated structure attains maximal response for acetone in contrast to other vapors examined. The study of ambient-effect on the device shows that it out-performs in oxygen ambient. A catalytic oxidation mechanism for detection of acetone with a model based upon Langmuir law of adsorption and Frenkel–Poole theory of electronic emission for the description of sensing behavior and vindication of experimental results have been proposed.

1. Introduction

The development of a convenient yet efficient device for detection of hydrocarbon-vapors (viz. ethanol, acetone, ethylene, trichloroethylene (TCE) etc.) and hydrogen have received urgent demand in pharmaceuticals and chemical industries. Acetone oxidizes in air severely and, thereby, depletes the oxygen-content of atmosphere playing as noxious air-pollutant. TCE, a major ground water pollutant, is responsible for hazardous water-borne diseases. It is, therefore, necessary to judicious monitoring and controlling of such pollutants by developing an electronic device which may be utilized as portable detector.

Recently, for detecting such hydrocarbons, different metal-oxide semiconductor materials such as ZnO, SnO_2, WO_3 and TiO_2 etc. are utilized for sensing film as they offer low cost, long-lasting, better sensitivity as well as selectivity over conventional solid state gas sensor [1–6]. Metal Oxide Semiconductor (MOS) structure based on Silicon dioxide (SiO_2) and Titanium dioxide (TiO_2) with catalytically active materials (Pd, Pt, Ni etc.) as electrode yielded better sensitivity for hydrogen and hydrogen containing molecules [7–10]. TiO_2, in the rutile phase, has distinctive importance in the gas-sensing field due to its non-poisonous nature and offering maximum polarizability in contrast with SiO_2. Several investigations have been carried out taking TiO_2 as sensing material in the form of thick/thin and nanocrystalline film for detection of alcohols, hydrogen, ethylene and trimethylamine etc. [11–14].

The gas-sensing behavior of thin film is characterized by conductivity/capacitance change, if film-surface is allowed to interact with reducing or oxidizing incoming gases/vapors. Since acetone is one of the serious air-pollutants, it must be decomposed to less harmful gases/compounds. Various studies have been performed to investigate the possible reaction-mechanism during oxidation of acetone on TiO_2 [15,16]. The role of most reactive oxygen anion (O^-) over TiO_2 surface in presence of light resulted photo-catalytic oxidation of organic compounds [17,18].

A grided $Pd/TiO_2/Si$ MOS structure (Pdtisin sensor) have been fabricated by Yadava et al. [19,20] to detect hydrogen gas. In the present work, the Pdtisin sensor is investigated for detecting hydrocarbons such as ethanol, acetone and TCE in different ambient (O_2, N_2 and Ar). Measurements revealed that MOS sensor displayed maximal response toward acetone in oxygen ambient among other vapors detected. The paper is organized as follows: In Section 2, a brief description of device fabrication is given. The change in capacitance of the device, its analysis and sensing mechanism is discussed in Section 3. In the Section 4, a model based upon the theory of Frenkel–Poole emission for sensing behavior of Pdtisin sensor is proposed and corroborated by observed results. The last section concludes the findings.

2. Experimental detail

The Pdtisin sensor has been fabricated by evaporating TiO_2 over a thoroughly cleaned p-type <111> silicon wafer having resistivity 3–6 Ω-cm. Resistive heating technique is used to deposit TiO_2 film at partial pressure of 6.7×10^{-3} Pa in a Hind-Hivac vacuum coating unit [20]. The thickness of TiO_2 film was about 0.6 μm (1 μm = 10^{-6} m) .Th

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