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Pd-Functionalized ZnO:Eu Columnar Films for Room-Temperature Hydrogen Gas Sensing: A Combined Experimental and Computational Approach

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Abstract

Reducing the operating temperature to room temperature is a serious obstacle on long-life sensitivity with long-term stability performances of gas sensors based on semiconducting oxides, and this should be overcome by new nanotechnological approaches. In this work, we report the structural, morphological, chemical, optical, and gas detection characteristics of Eu-doped ZnO (ZnO:Eu) columnar films as a function of Eu content. The scanning electron microscopy (SEM) investigations showed that columnar films, grown via synthesis from a chemical solutions (SCS) approach, are composed of densely packed columnar type grains. The sample sets with contents of ~0.05, 0.1, 0.15, and 0.2 at% Eu in ZnO:Eu columnar films were

studied. Surface functionalization was achieved using PdCl2 aqueous solution with additional thermal annealing in air at 650 °C. The temperature-dependent gas-detection characteristics of Pd-functionalized ZnO:Eu columnar films were measured in detail, showing a good selectivity toward H2 gas at operating OPT temperatures of 200–300 °C among several test gases and volatile organic compound vapors, such as methane, ammonia, acetone, ethanol, *n*-butanol, and 2-propanol. At an operating temperature OPT of 250 °C, a high gas response *I*gas/*I*air of ~115 for 100 ppm H2 was obtained. Experimental results indicate that Eu doping with an optimal content of about 0.05–0.1 at% along with Pd functionalization of ZnO columns leads to a reduction of the operating temperature of the H2 gas sensor. DFT-based computations provide mechanistic insights into the gas-sensing mechanism by investigating interactions between the Pd-functionalized ZnO:Eu surface and H2 gas molecules supporting the experimentally observed results. The proposed columnar materials and gas sensor structures would provide a special advantage in the fields of fundamental research, applied physics studies, and ecological and industrial applications.