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An enhanced butanone sensing performance of $Er_{0.7}Yb_{0.3}FeO_3$ material with the proper electronic structure

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Abstract: $Er_{1-x}Yb_xFeO_3$ (x=0, 0.3, 0.7, 1) sensing materials were synthesized via sol-gel method and annealing. The obtained porous $Er_{0.7}Yb_{0.3}FeO_3$ solid solution had the highest response value (Rg/Ra=2.8) to 0.5ppm butanone and the optimal selectivity compared with $Er_{1-x}Yb_xFeO_3$ (x=0, 0.7, 1) sensing materials. The combination of Er^{3+} and Yb^{3+} rare-earth elements in A site of $AFeO_3$, and proper proportion of Er to Yb make contribution to gas sensing properties of $Er_{0.7}Yb_{0.3}FeO_3$ because they create the proper structure which has more electronic density of states near the Fermi level and the proper band-gap structure in $Er_{0.7}Yb_{0.3}FeO_3$ according to the first-principle calculation results and UV-Vis diffusion spectra. Therefore, the better electronic structure of $Er_{0.7}Yb_{0.3}FeO_3$ increases the amount of absorbed oxygen species on surface of materials, which is proved by the XPS results, and then enhances the response to target gas. In conclusion, $Er_{0.7}Yb_{0.3}FeO_3$ has the great potential as gas sensing material used in detecting butanone and other hazardous gases.

Key words: $Er_{1-x}Yb_xFeO_3$, Butanone gas sensor, Electronic structure, Sol-gel

1. Introduction

Gas sensors play a significant role in environment pollutants monitoring, chemical process monitoring and health care [1]. They can rapidly respond to such hazardous gases as butanone, even in low concentration, by sending the electronic signals [2]. They also have the advantage of low cost and energy efficiency [3]. As a kind of advanced functional material, rare-earth ferrites has a great potential for being used in gas sensor[4-6], solar cells[7], catalysis[8, 9] and superconductors[10]. Of all the gas sensing materials having been studied so far, rare-earth ferrites with perovskite-type crystal structure have aroused great interests among researchers due to their stabilities at high temperatures and in chemically aggressive atmospheres[11]. Meanwhile, the advantage of fast oxygen ion mobility and catalytic properties in rare-earth oxide is beneficial to gas sensing performance of materials [12]. Furthermore, the research of rare-earth ferrites with the magnetism may provide the research basis for the relationship between the magnetism and gas sensing properties [13].

Previous researches have shown that when the A site is placed with various rare-earth elements, $AFeO_3$ can present different gas sensing properties. Take the results of the some recent studies for example. Yolk-shell $LaFeO_3$ microspheres had a response of 25.5 towards 100 ppm acetone at 225 °C [14]. Hollow $PrFeO_3$ nanofibers exhibited a high response of 6 to 10 ppm acetone at a low