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Absorption behavior of lattice oxygen in $Ce_{0.8}Y_{0.2}O_{2-\delta}$ at intermediate temperature

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Abstract: The absorption behavior of lattice oxygen for $Ce_{0.8}Y_{0.2}O_{2-\delta}$ (YDC) crystal was investigated. Combined with TG-DSC, XRD, Raman and XPS characterization, lattice oxygen absorption occurs at intermediate temperature (from 500 to 800 °C), which is related to the oxygen vacancies consumption, and no phase change is observed in this process. In electric conductivity relaxation (ECR) experiment, prolonged oxygen diffusion process is observed above 600 °C, which may be caused by oxygen absorption process. And through ECR experiments, the bulk diffusion coefficient D_{chem} and surface exchange coefficient K_{ex} for YDC dense sample are measured as 6.5×10^{-5}–2×10^{-4} cm^2/s and $K_{ex}=2\times10^{-4}$–9×10^{-4} cm/s at intermediate temperature range.

Keywords: Y doped CeO_2; ECR; XPS; Oxygen vacancies; Oxygen absorption; Rare earths

1. Introduction

Intermediate temperature solid oxides fuel cell (IT-SOFC) operating at 500-800°C has been considered as one of the promising techniques in new energy field, which attracts much attention[1–3]. CeO_2-based materials, such as lanthanoid doped CeO_2,are usually investigated as electrolyte in IT-SOFC due to their higher ion conductivity[4-6]. The effect of doped rare earth has been extensively studied by experimental methods and theoretical methods [7, 8]. Nakayama et al. reported that the electronic was strongly associated with oxygen vacancies in the ceria by the density functional theory+U (DFT+U) method[9], which lowered the migration energy of the oxygen vacancies during the ionic transition process and increased the diffusivity of the oxygen vacancies. In the doped ceria materials, the binding energy of oxygen vacancy clusters would have significant change caused by the dopant cations, which consequently influence the oxygen migration process. Besides, transformation between Ce species and oxygen vacancies is also an important factor for the catalytic property applications[10-12], which may influence the performance of doped ceria significantly.

In the Y-doped CeO_2 materials, the nano-particle dopants have more weak bonded structure and less constrained bonding environment than pure ceria materials[13], which resulted in more active oxygen ionic and higher electrical conductivity[14]. The interaction between charged defect and trivalent dopant at intermediate temperature strongly influenced the electric property and the formation enthalpies[15]. Besides, the weight increase of YDC at intermediate temperature was observed in many researches, but scarcely well explained[16]. However, this information is related to the oxygen vacancies involved reaction at intermediate temperature, which has important effect on the electrical performance for YDC.

Therefore, in this paper, oxygen absorption behavior and oxygen vacancies variation in YDC were characterized in detail by TG, XRD, Raman and XPS, respectively, while the bulk diffusion coefficient D_{chem} and surface exchange coefficient K_{ex} for YDC were measured by electric conductivity relaxation (ECR) method. Based on these studies, the interrelation between oxygen absorption behavior and oxygen vacancies diffusion was suggested for YDC at

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