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PROCEEDINGS

Effect of lanthanum doping on the ceria fluorite structure and its relationship with transport properties

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Doped ceria and its solid solution are popular materials widely investigated in energy conversion and electrochemical devices. It has a cubic fluorite structure and doping with La^{3+} changes to a disordered fluorite and a C-type structure. Moreover, the doping level offers a path to tune the defect chemistry for applications in several fields.[1] In this work, we investigate solid solutions of La-doped ceria ($La_xCe_{1-x}O_{2-x/2}$) with x from 0 to 50 at.% compressed into pellets to investigate the electrical properties and its correlation with defect chemistry and crystal structure. The transport properties were studied via electrochemical impedance spectroscopy in air and different p_{O2}. The findings show that electrical conductivity increases from 0 to 5 at.%, and then remains constant up to 15 at.%. However, beyond 20 at.%, it starts to decrease. This trend can be explained by the formation of vacancies formation.[2] For lower levels of lanthanum doping, the creation of vacancies improves conductivity. However, at higher concentrations (>20 at.%), the increase of oxygen vacancies leads to the formation of dopant-vacancy clusters. This process arises from the Coulomb interaction between vacancies and local lattice relaxation in the crystal. The increase in activation energies above 20 at.% indicates higher resistance to defect migration. X-ray powder diffraction indicated the presence of only one phase with increased strain and expansion of lattice parameters, as determined through Rietveld refinement. Raman spectroscopy indicated structural changes in the fluorite structure, including the emergence of a C-type phase. Additionally, it detected local symmetrical breaking and vibrational changes in the structure due to the formation of oxygen vacancies.

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1. Trindade et al. ACS Appl Nano Mater 2022, 5 (7), 8859.
2. Zamudio-García et al. Inorg Chem 2019,