Understanding the effect Ce and Zr to Explain Chemical Expansion Difference between Y-Doped $SrCeO_3$ and $SrZrO_3$

Takaya Fujisaki [(a)], Aleksandar Tsekov Staykov [(a)], Yuhang Jing [(b)], Kwati Leonard [(a)], Narayana R Aluru[(b)], Hiroshige Matsumoto[(a), (c)*]*

[(a)]International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University, 744 Motooka, Nishi-Ku, Fukuoka, 819-0395, Japan
[(b)]Department of Mechanical Science and Engineering, University of Illinois at Urbana−Champaign,Urbana, Illinois 61801, United States
[(c)]Next-Generation Fuel Cell Research Center (Next-FC), Kyushu University, 744 Motooka, Nishi-Ku, Fukuoka, 819-0395, Japan

*E-mail of the Corresponding Author: fujisaki.takaya.485@m.kyushu-u.ac.jp

Abstract

Aliovalent cation-doped perovskite-type oxides (ABO_3) exhibit proton conductivity originating from the hydration of oxide ion vacancies [1]. The hydration reaction is accompanied by structural deformation, i.e. chemical expansion. The chemical expansion may lead to mechanical failure in electrochemical devices, and thus it is necessary to understand the causes of this process at the atomic scale. In this study, the chemical expansion behaviors of Y-doped strontium cerate and zirconate were comparatively investigated. High-temperature X-ray diffraction and thermogravimetric analysis revealed that the cerate exhibits larger chemical expansion. In addition, density functional theory calculations revealed that size of oxide ion vacancies, and covalency (See Figure 1) between *B*-site and oxygen played important roles to understand the chemical expansion difference [2].

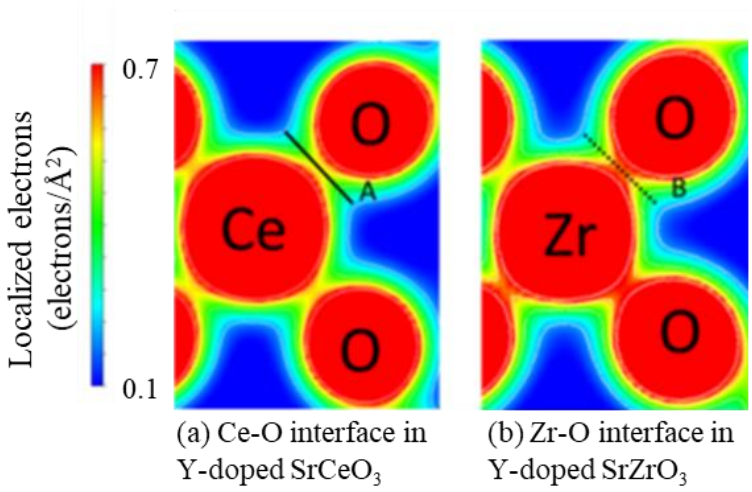

Figure1 Covalency difference between Y-doped $SrCeO_3$ and $SrZrO_3$ obtained by density functional theory

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References
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