

Theoretical and Experimental Study on Mechanical and Electrochemical Properties of Proton Conducting Oxides Originated from Hydration and Influence of Interfaces

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Name

論 文 名 : Theoretical and Experimental Study on Mechanical and Electrochemical
Properties of Proton-Conducting Oxides Originated from Hydration and
Influence of Interfaces

(プロトン伝導性酸化物の水和に起因する機械的・電気化学的特性と界面の影響
に関する理論・実験研究)

Title

区 分 : 甲

Category

論 文 内 容 の 要 旨

Thesis Summary

This thesis consists of 6 chapters in total. 1st chapter firstly introduces the research field of solid state ionics. The solid state ionics is covering the research field of proton conducting oxides this thesis mainly focuses on. In the 2nd chapter, to evaluate the physical properties of proton conducting oxides, this study especially performs the first principle calculations as research methods from chapters 3 to 5, and the details of the calculation method is theoretically introduced. 3rd chapter explains the results of the study on chemical expansion by hydration of proton conducting oxides. For proton conduction, hydration must take place in the oxide-ion vacancies in the proton conducting oxides. This chapter clarifies how Ce and Zr contribute to chemical expansion in proton conducting oxides. 4th chapter investigated why the hydration of proton conducting oxides takes place by first principles calculation. Even though oxygen vacancies exist among many metal oxides, the hydration reaction does not take place in all of them. The study in this chapter pays attention to bulk Y doped SrZrO₃ and Y stabilized ZrO₂, which have oxide-ion vacancies. This research discusses the origin of hydration from the viewpoints of covalency between Zr-O and Ce-O. In 5th chapter, it attempts to explain the effect of platinum nanoparticles in proton conducting oxides by first principles calculation. The effect of the interface between the platinum nanoparticles and a proton conducting oxide was investigated for the defect equilibrium of protons. In 6th chapter, experimental investigations were conducted on anomalous electric conductivity observed in dry hydrogen.

This thesis has two topics in appendixes which are Appendix A and B. Firstly, Appendix A shows a social background for the energy supplying system combining renewable energy and hydrogen. Appendix B introduces a concept of “Green Paradox” and evaluates if the Green Paradox takes place in Japan.