

## 【Grant-in-Aid for Specially Promoted Research】

### Science and Engineering (Engineering)



#### Title of Project : Creation of Novel High Performance Catalyst Tailored by Chemo-mechanical Effects

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Research Project Number : 16H06293 Researcher Number : 80184555

Research Area : Engineering

Keyword : Catalyst, Chemo-mechanical effects, Nano size effects, Ion conductivity

#### 【Purpose and Background of the Research】

Although it is known that chemo-mechanical stress can have a large influence on many materials properties, especially ionic conductivity [1], its influence on surface activity and catalytic activity has not yet been studied in detail. In a previous study, we showed that the tensile stress caused by chemical relaxation can significantly enhance bulk oxide ion conductivity as well as surface activation to oxygen dissociation. Building on these promising results, the proposed study will systematically investigate the effects of chemo-mechanical strain on the surface chemistry and associated catalytic activity of the oxide. Since significant increases in activity are necessary in many applications, the influence of such strain effects on the performance of air electrodes in fuel cells, for NO decomposition reactions, for diesel particulate matter (PM) oxidation catalysts, and even photocatalytic reactions, will be investigated.

The originality of this study lies in harnessing these chemo-mechanical strain effects to develop a new class of catalysts. The present study seeks to apply an approach which has not yet been explored, to increase the diffusivity of lattice oxygen (or oxygen vacancies) to these important area.

#### 【Research Methods】

Details of this research are 1) To tailor chemo-mechanical strain in materials such as perovskite, or oxygen deficient fluorite, oxides. For this purpose, we will use laminated epitaxial films with nm thickness and controlled mismatch between lattice sizes. A second approach will involve the dispersion of metal or metal nitrate nano-particles having different thermal expansion in the oxide matrix (Figure). 2) The effect of such strain on surface chemistry, catalytic activity, or electrochemical activity will elucidated. 3) Change in gas adsorption or desorption properties ( $O_2$ ,  $NO$ , and  $H_2$ ) will be evaluated, and the relationship between changes in structure (by neutron diffraction, EXAFS, TEM, XPS etc.) and properties (charge carrier density, spin state, oxygen non-stoichiometry) will be discussed from chemo-mechanical strain effects. 4) The mechanism

for beneficial effects of chemo-mechanical strain on surface chemistry and activity will be analyzed based on first principles DFT calculation. From this study, we expect to demonstrate a new concept for catalyst design.

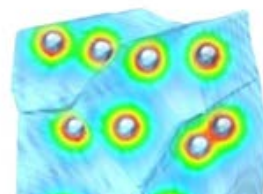


Fig. Image of nano strain effects formed by dispersion of nano particle.

#### 【Expected Research Achievements and Scientific Significance】

We will investigate the effect of lattice strain on NO decomposition, low temperature diesel PM oxidation, and photocatalytic activity, which are also important applications to address environmental issues. Therefore, the topic studied in this project will have a broad impact for energy and environmental applications, and significantly benefit society.

#### 【Publications Relevant to the Project】

J. Druce, H. Tellez, M. Burriel, M. Sharp, L. Fawcett, S. N Cook, D. McPhail, T. Ishihara, H. H. Brongersma and J. A Kilner, *Energy & Environmental Science*, 7(11), 3993-3599, (2014)

【Term of Project】 FY2016-2020

【Budget Allocation】 380,700 Thousand Yen

#### 【Homepage Address and Other Contact Information】

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