

## First-principles Study of Adsorption Properties on Ni/YSZ Surface

OShixue. Liu<sup>1,2</sup>, Takayoshi Ishimoto<sup>1,2</sup>, Michihisa Koyama<sup>1,2,3</sup><sup>1</sup>INAMORI Frontier Research Center, Kyushu University  
(744 Motoooka, Nishi-ku, Fukuoka 819-0395)<sup>2</sup>CREST, Japan Science and Technology Agency

(K's Gobancho 7, Gobancho, Chiyoda-ku, Tokyo 102-0076)

<sup>3</sup>International Institute for Carbon-Neutral Energy Research, Kyushu University  
(744 Motoooka, Nishi-ku, Fukuoka 819-0395)

## 【Introduction】

Ni/YSZ is a typical material of solid oxide fuel cell anode. To understand the anodic reaction mechanism in atomic scale, density functional theory (DFT) method is needed. There are few DFT research about the reactions on Ni/YSZ three phase boundaries (TPBs) [1]. In the present study, a periodic model includes Ni (metal) and YSZ (ceramic) was built. Adsorption properties of H, O, OH, were examined on different sites, near or on the TPB sites. The surface diffusion process will also be discussed.

## 【Method】

For YSZ structure, a slab model with oxygen terminated (111) surface,  $Zr_{46}Y_8O_{104}$ , was built. The slab includes 6 layers of O and 3 layers of Zr/Y. A Ni ridge with 36 atoms was put on the YSZ slab. The contact interface between Ni and YSZ is (100) for Ni and (111) for YSZ. In the TPB area, the surfaces are both (111) surfaces. Fig. 1 shows the structure of the model. DFT method (VASP code) was used to calculate the electronic properties of the structures. GGA/PBE functional was chosen for all the elements and the cutoff energy of plane wave was set to 400 eV.

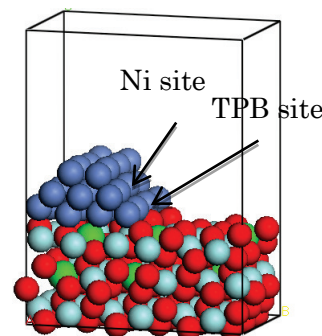


Fig. 1 The Ni/YSZ model with adsorption site. Color of balls, blue: Ni, red: oxygen, green: yttrium, cyan: zirconium.

## 【Results and Discussion】

The species of H, O and OH were put on Ni site near TPB or TPB site and structures were optimized. The adsorption energy is shown in Table 1, comparing with the result on pure Ni(111) surface. The adsorption energy of H and OH are almost same at Ni site of Ni/YSZ model and at pure Ni(111) surface model. For the species on TPB site, the adsorption energy of H changes a little from Ni site, but OH changes 0.8 eV, which is big enough to affect the reaction barrier of oxidation reaction in SOFC.

Table 1 The adsorption energy (eV) of H, O and OH on Ni site and TPB site of Ni/YSZ.

	H		O		OH	
	Ni	TPB	Ni	TPB	Ni	TPB
Ni/YSZ	-0.56	-0.54		-2.24	-3.50	-4.28
Pure Ni [2]	-0.54		-2.33		-3.51	

## 【Acknowledgement】

Activity of INAMORI Frontier Research Center is supported by KYOCERA Corporation.

## 【References】

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