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Diffusion Pathways of Hydrogen for Solid Oxide Fuel Cells Anode Using Reactive Molecular Dynamics Simulation

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【Introduction】

Solid oxide fuel cell (SOFC) is an electrochemical device that converts the energy of a chemical reaction directly into electrical energy. As SOFC systems typically operate at high temperatures between 700 and 1000 ºC, consequently H-atoms may diffuse from Ni to the YSZ surface. Herein, we studied the diffusion pathways of H atoms either surface or the bulk path into the Ni in the range of SOFC operating temperature and eventually calculated diffusion barrier.

【Method】

We used the ReaxFF potential [1] to investigate the interaction between H and Ni surface. ReaxFF is based on the bond order/bond distance relationship introduced by Abell and applied to hydrocarbons by Brenner. A more detailed description of the force field can be found in reference 2.We perform constant temperature (NVT) MD simulations. The H atoms are set on the Ni(100)/Ni(111) surface. Ni(111), which is the most stable Ni surface and the most abundant surface facet in typical nickel catalysts. Ni(100), which has a higher surface energy and is also present in nickel catalysts. The system temperature range of 973-1373 K was considered for surface/bulk diffusion of H atoms. We adopted the LAMMPS package for reactive MD simulations.

【Results and Discussion】

From 973 to 1073 K, most of the H atoms stay on the surface, while a couple of H atoms move into the bulk region. From 1173 to 1273 K, several H atoms diffuse into the bulk region. In case of 1273 K, 30 % H atoms are found into the bulk region. The H migration from surface into the bulk increases with increasing temperature. The number of H atoms from surface into the bulk is greatly influenced when temperature reaches to 1173 K, but the majority is always surface pathway. H diffusion into the bulk may vary depending on Ni surfaces. Figure 1 shows the Arrhenius plots of the diffusion coefficient. Diffusion barrier of H into bulk is calculated higher than the surface pathway.

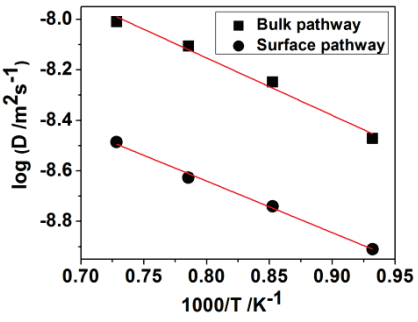

Figure 1. Arrhenius plots of the diffusion coefficients for H.

【Acknowledgement】

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【References】

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