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Size Effect of YSZ Nanoparticles on Sintering of Ni Nanoparticles in Ni/YSZ Anode of Solid Oxide Fuel Cell via Multi-Nanoparticle Molecular Dynamics Simulation JINGXIANG XU, YUJI HIGUCHI, NOBUKI OZAWA, MOMOJI KUBO, Fracture and Reliability Research Institute, Graduate School of Engineering, Tohoku University — Sintering of Ni nanoparticles leads to the degradation of a Ni/YSZ porous electrode of solid oxide fuel cell. We reported that the YSZ nanoparticle framework plays an important role in inhibition of sintering by using our multi-nanoparticle molecular dynamics simulation method [1]. Size of YSZ nanoparticles affects the framework of YSZ nanoparticles and changes the sintering in Ni/YSZ porous structure. However, the mechanism of different sintering behavior by changing the size of YSZ nanoparticle has not been revealed. In this study, we used our multi-nanoparticle molecular dynamics simulation method to investigate the size effect of YSZ nanoparticles on the sintering of Ni nanoparticles in the Ni/YSZ porous structure. Then, Ni nanoparticles make contact with each other and the sintering proceeds by growth of contact area between Ni nanoparticles when YSZ nanoparticles are large. In contrast, the sintering of Ni nanoparticles is suppressed when YSZ nanoparticles are small. It is found that interfacial area between Ni and YSZ in the small YSZ nanoparticles model is larger than that in the large YSZ nanoparticles model. Thus, the movement of Ni nanoparticles is disturbed, and the sintering is inhibited. [1] J. Xu et al., J. Phys. Chem. C 117 (2013) 9663.

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