Electronic supplementary infomation

Prospects of on-chip fuel cell performance: improvement based on numerical simulation

Satoshi Tominaka,[1]‡ Sousuke Ohta,[1] Tetsuya Osaka[1]* and Richard Alkire[2]

[a]*Department of Applied Chemistry, Graduate School of Advanced Science and Engineering, Waseda University,Tokyo 169-8555, Japan.*
[b]*Department of Chemical & Biomolecular Engineering, University of Illinois, Urbana, IL 61801, USA*
‡*Current affiliation: World Premier International (WPI) Research Center for Materials Nanoarchitectonics (MANA), National Institute for Materials Science (NIMS), Namiki 1-1, Tsukuba, Ibaraki 305-0044, Japan. E-mail: TOMINAKA.Satoshi@nims.go.jp*
** E-mail: osakatets@waseda.jp*

Details on the mesh for the simulation

Extended mesh

- Number of degrees of freedom: 124533

Base mesh

- Number of mesh points: 9133
- Number of elements (Triangular): 17856
- Number of boundary elements: 688
- Number of vertex elements: 14
- Minimum element quality 0.5841
- Element area ratio 0.0033

Figure S1 Created mesh for simulation.

Rough estimation of the active area of the PtRu electrode

We used CO stripping measurements to evaluate electrochemically active surface area of almost the same PtRu electrode, by following the method reported by Takasu *et al.* [Electrochem. Commun. 6 (2004) 480]. The electrode we used for the test was deposited from a similar deposition solution but containing 2 M HCl. Consequently, the roughness factor, which is defined as the ratio of the electrochemically active surface area to the geometrical one, was calculated as *ca*. 30. By comparing the charge of the CVs of this electrode and the one used in this work scanned in 0.5 M H_2SO_4 deaerated with N_2, we roughly estimated the roughness factor of the electrode used in this work as *ca*. 25 for the latter. Detail data will be submitted in a future paper.

The conditions for the CO stripping voltammetry are as follows. (*i*) CO was first adsorbed at 0.1 V vs. Ag/AgCl for 40 min in 0.5 M H_2SO_4 purged with CO gas at 60°C. (*ii*) The CO gas was removed by bubbling with Ar for 40 min. (*iii*) Cyclic voltammograms were scanned in the potential range of 0.1 to 0.8 V at 10 mV s^{-1}. (*iv*) From the stripping charge, electrochemically active surface area was calculated as described the reference [Electrochem. Commun. 6 (2004) 480].