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Computational prediction of nano-electrode structures by using highly ordered ionomers for statistical morphology analysis

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New concepts of nano-electrode structures for advanced electrochemical energy application are proposed by using highly ordered ionomer structures. Catalyst utilization of the highly ordered ionomer catalyst layers is predicted by statistical morphology analysis [1, 2] and compared with both conventional and VACNT catalyst layers. For the detailed morphological analysis, a series of multi-component distributions at a 95% confidence level are randomly generated to deduce the statistical variations of effective transport paths of ternary catalyst components. In the highly ordered ionomer catalyst layers, all of the ionomers are successfully interconnected and therefore, all ionomers can be utilized as ionic current paths. Numerical results reveal that despite the relatively poor interconnections of the electric and mass transport paths (49.3% and 86.1%, respectively), the statistical average catalyst utilization of highly ordered ionomer catalyst layers is significantly improved when compared to conventional catalyst layers. For the conventional electrodes of 30 vol.% Pt/C, 33 vol.% ionomer, and corresponding porosity of 37%, the average effective catalyst utilization is estimated to be 27.5%. However, for the highly ordered ionomers, the average effective catalyst utilization is predicted to be 34.7%, which is remarkably higher than that of the conventional catalyst layers with the same catalyst composition. It is also found that the ionomer volume fraction of the ordered ionomer catalyst layers can be considered as a catalyst utilization determining factor and a moderate amount of ionomers are necessary to enhance electrochemical performance.

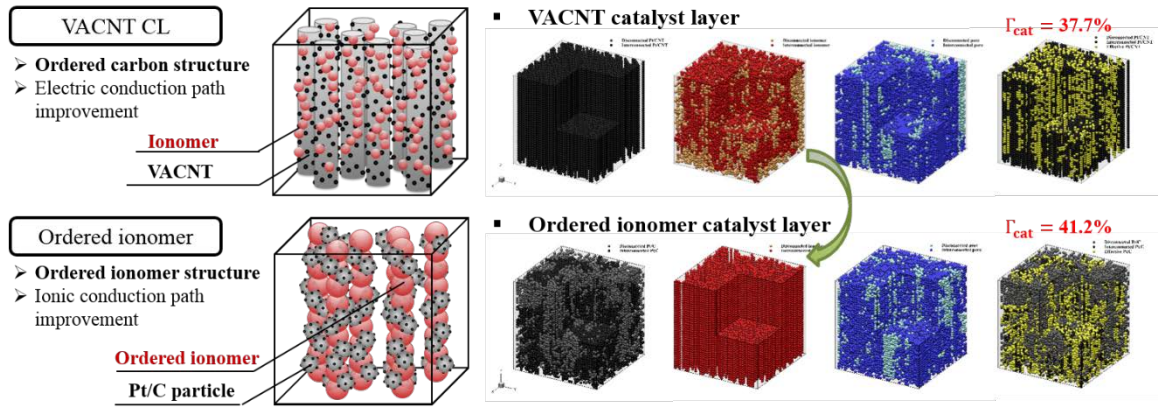

Figure 1: Schematic diagram and three-dimensional morphological structures of VACNT and ordered ionomer catalyst layers

REFERENCES

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