Quantitative relationship between 3D structure-ionic conductivity by topological analysis

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In recent years, topological data analysis has rapidly grown for evaluating the structure shapes in materials science.[1] A particularly important application is quantitatively correlating the structure-property relationship using Betti numbers, which is helpful for the materials design.[2-4] Betti numbers are topological invariants to quantitatively describe the feature of an object. The calculation of Betti numbers can be performed computationally from 2-dimensional or 3-dimensional (3D) images. However, there are few reports on the Betti numbers for the transmission electron microscopy (TEM) images of nanomaterials.[5] In this work, we combined scanning TEM (STEM) tomography reconstruction with homology analysis to quantitatively relate the 3D structure and ionic conductivity of self-assembled Pt/CeO_2 nanocomposites.

Self-assembled Pt/CeO_2 nanocomposites were prepared by the annealing of the Pt_5Ce alloy in a reactive atmosphere, and different morphologies of the composites were made by changing the annealing temperature. The 3D structure of the composites was reconstructed by high-angle annular dark-field–STEM tomography and post-processing. Betti numbers were used to describe different composites in topological view. Specifically, Betti 0 indicates the number of CeO_2 phases, Betti 1 is the number of Pt tunnels, and Betti 2 is the number of Pt cavities. The ionic conductivity measured by impedance spectroscopy was interpreted by two parameters: activation energy E and pre-exponential factor $\ln \sigma$. We demonstrate that the trends of E and $\ln \sigma$ as a function of annealing temperature are consistent with that of Betti 0, which suggests the important role of CeO_2 phase number to the ionic conductivity. The higher connectivity of the CeO_2 phase (represented by lower Betti 0) has a higher value of E and $\ln \sigma$ for the self-assembled Pt/CeO_2 nanocomposites. This finding provides a suitable way to build a quantitative relationship between the 3D structure-ionic conductivity of self-assembled composites.

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