عنوان مقاله:

Monte Carlo Simulation of Three Phase Boundary Length in Cermet Anode of Solid Oxide Fuel Cells

محل انتشار:

کنفرانس بین المللی پژوهش در علوم و مهندسی (سال: 1395)

تعداد صفحات اصل مقاله: 12

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خلاصه مقاله:

A numerical model for calculating active three phase boundary length in the cermet structure of Ni-YSZ composites is developed to gain insight into the important microstructural behaviors of solid oxide fuel cell (SOFC) anodes. By combining Monte Carlo techniques of reconstructing random structures with experimental studies of detecting three phase boundaries (TPB), a SOFC anode can be modeled in three dimensions and the density of TPB in its structure can be calculated. To study the effect of porosity and solid phases, simulations were performed for different porosities and nickel contents. Two different algorithms is used to generate the anode structure, one simply based on uniformly distributed random numbers, the other with and additional random walk at each step. The structures generated with random walker are more likely to be the case that happens in reality. The results of the simulation confirmed that TPB density strongly depends on the porosity and the volume fraction of components of anode. The results show that the maximum TPB density happens at equal volume fraction of solid components and the porosity of 30-35%. The methodology can be used to optimize the anode structure of SOFCs and improve the performance of the system.

کلمات کلیدی:

Solid Oxide Fuel Cell, Anode, Monte Carlo Simulation, Three Phase Boundary, Porosity