Simulation of the Impedance Response of Materials with More Than One Electrical Path

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Abstract

1. Introduction

Polycrystalline single phase materials often display electrical properties that are a function of their grain size. Impedance spectroscopy, an alternating current technique is ideal for detecting the presence of more than one current path and has been used for many years[1,2]. However, it is proposed here that it may be possible to use concepts developed for two phase composites, to unravel the complexities of their electrical response as function of grain size and/or grain boundary thickness. The finite element model being used here was first developed to represent an ordered insulator-conductor composite with a segregated network microstructure [3].

2. Use of COMSOL Multiphysics®

In this study, we used a finite element approach to solve the electric potential in the AC environments for an idealized two-phase microstructure as shown in Figure 1. The faceted grains represent the main material phase and the boundary region has finite thickness and distinct electrical properties that may or may not percolate with itself. The steps used include: (1) Selecting the AC/DC Module in the COMSOL Multiphysics® software, (version 4.4), (2) Defining the electrical properties inside the grains and the grain boundaries, (3) Solving and finding the electric field distributions and (4) Using postprocessing capabilities in the COMSOL software to determine the impedance response.

3. Results

Figure 2 illustrates simulated equivalent circuit complex impedance spectra when the two electrical paths are in series [4]. It is clear that changes in the conductivity of the main grains may or may not be detected, depending on whether the grain boundaries are more or less conducting than the matrix grains.

Assuming a situation where the grain boundaries are more conducting than the matrix grains, FEA simulations revealed that if the grain boundaries are allowed to percolate, the complex impedance spectra may be dominated by the properties of the matrix grains or the grain boundaries. In order to evaluate these effects, percolated and unpercolated structures using the same grain size and grain boundary area were simulated. In Figure 3(a), it can be seen that

unpercolated grain boundaries give rise to perfect semicircles as would be expected from a simplified equivalent circuit analysis of two parallel RC circuits in series. However, in Figure 3(b), it is clear that if the grain boundaries form a percolated path that both the matrix grain semicircle and the grain boundary semicircle undergo shape changes. Similar shape changes in the complex impedance are seen when the radius of the grains or grain boundaries is varied by several orders of magnitude while the grain boundary phase percolates (not shown).

4. Conclusions

The FEA simulations have revealed that complex impedance semicircle shapes are very sensitive to the size and properties of the matrix grains and grain boundaries. Combining equivalent circuit and FEA analysis will be very powerful in helping to understand the behavior of complex heterogeneous materials, as well as for any material that is undergoing a phase change or any other process that can affect the behavior of the grain boundaries separately from the matrix grains.

Reference

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[2] J. Fleig, B. Rahmati, S. Rodewald and J. Maier, "On the Localized Impedance Spectroscopic Characterization of Grain Boundaries: General Aspects and Experiments on Undoped SrTiO3," J. Eur. Ceram. Soc. vol. 30, pp. 215–220, 2010.

[3] Y. Jin and R.A. Gerhardt, "Prediction of the Percolation Threshold and Electrical conductivity of Self-Assembled Antimony-Doped Tin Oxide Nanoparticles into Ordered Structures in PMMA/ATO Nanocomposites, " ACS Appl. Mater. Interfaces, vol. 6, pp. 22264 –22271, 2014.

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Figures used in the abstract

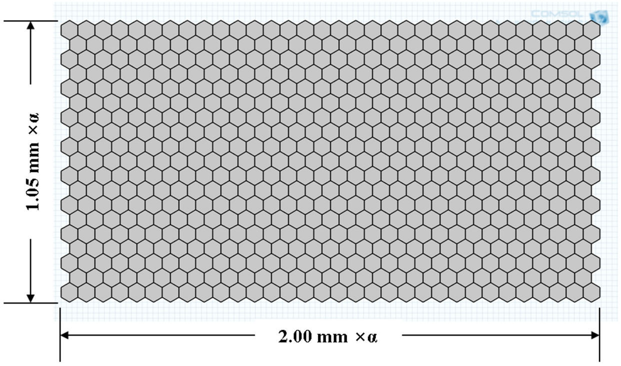

Figure 1: Schematic of the geometric model used for the simulations.

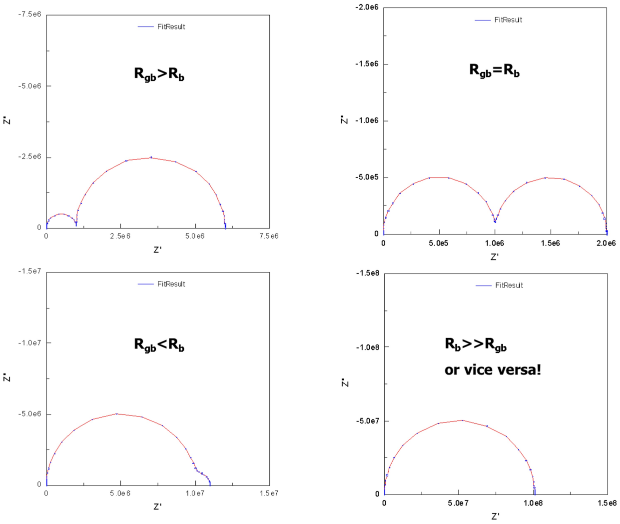

Figure 2: Simulated complex impedance spectra when the electrical response of the boundaries is equal, larger or smaller than the main phase grains. Modified from ref[4].

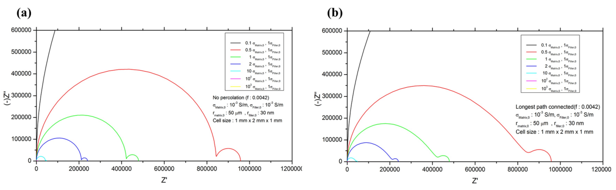

Figure 3: FEA simulated complex impedance spectra for an unpercolated material (a) and a percolated material (b) where ratio of the conductivity of the matrix grains is varied. It is clear that the percolated path contributes to modifying the electrical response.