Microstructure based numerical simulation of microwave sintering of specialized SOFC materials

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Abstract

A project underway in the Energy Materials Group at NRC-ICPET has been investigating novel materials such as LaCoO3 or La2NiO4 for use as SOFC cathode materials. Owing to their more complex electrochemical properties, these classes of materials have proven to be good microwave susceptors (absorbers) and consequently are being subjected to structure consolidation via microwave sintering. Advantages of this method are lower energy input, the possibility of attaining higher sintering temperatures and finer control over the sintering path through continuously tunable microwave energy output.

In-house finite element software has been developed for simulating the sintering of porous ceramic materials. The original application was to demonstrate mechanisms whereby functionally gradient structures (in terms of grain size and porosity) could sinter without warping and cracking. This was at first glance counter-intuitive, but with overlapping grain size distributions, physical samples of such structures could be prepared without warping, whereas green bodies built up in distinct layers would warp and delaminate under sintering. The underlying model and numerical simulation were able to demonstrate that by using particle size distribution as a local field variable, the sintering rates in an FGM could be made fairly uniform with overlapping broad PSDs owing to the resulting ensemble of particle-particle interactions.

Microwave sintering is a promising technique for processing SOFC cathode materials. Microstructural non-uniformities are known to cause imperfect physical samples. Since the numerical simulation we have is capable of treating local microstructural features as well as anisotropy, the code is ideally suited to studying the sample processing parameters pointing to the preparation of robust, stable and defect-free SOFC cathode materials

The objective of the project is the explore processing parameters in order to determine suitable processing conditions and parameter ranges, to assess the suitability of certain powder compacts for microwave sintering, as well as identifying the range of microstructure properties that would benefit from microwavesin