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Chemo-thermo-mechanics of ion-transport ceramic membranes

Di Leo, Claudio, cvdileo@mit.edu; Anand, Lallit, MIT, United States

ABSTRACT

Perovskite ceramics with high oxygen ionic conductivity are important materials for ion-transport membranes (ITMs) for oxygen separation or syngas production, as well as for electrode materials in solid oxide fuel cells (SOFCs) which operate at high temperatures (~500–1000°C). These ceramics have the ability to be (reversibly) reduced at moderate partial pressures of oxygen, to produce high concentrations of oxygen ion vacancies. While these vacancies facilitate oxygen ion transport and oxygen surface exchange, they also lead to lattice volume expansion and mechanical stress --- a factor which is of critical importance in determining success or failure during the use of membranes made from these materials In order to optimize the design of ITMs and SOFCs, there is need for a theory and numerical simulation capability which couples chemical, thermal, and mechanical effects. Of particular importance is the specification of appropriate flux boundary conditions which account for the insertion (extraction) reactions at the boundaries—reactions which depend on the external partial pressure of oxygen, the local concentration of vacancies at the boundary, and the stress in the material. We have formulated such a coupled theory. The fully-coupled theory is implemented in the commercially available finite-element software Abaqus through the development of custom user-elements. Using this simulation capability we have studied the transport of oxygen ions through a representative ITM membrane. Our study shows the importance of stress on the diffusion of vacancies through the ITM, and also shows that a proper accounting for the effect of stress on the surface reactions is crucial in developing a model that can fit experimentally available data. We have also developed a simplified one-dimensional model that may be solved efficiently without the need for finite-element simulations. We have used our full finite element implementation to check the range of validity of our simple one-dimensional model. The simple one-dimensional model represents an important tool for the engineering design of ITM membranes since it is computationally inexpensive, and may thus be used to quickly simulate a variety of designs. We conclude by using our theory, its finite element implementation, and our simplified one-dimensional model to conduct a parametric study to determine the importance of various key design parameters which affect the performance of ITMs.