Designing Next-generation Electrolytes for Solid Oxide Fuel Cells

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Abstract

Concepts such as energy continue to develop our community and technological advancement. Being a vital role in modern day lifestyles, energy has come in many shapes and forms. But all forms are being adjusted to optimize their outputs and minimize their costs. A prime example of this is the Solid Oxide Fuel Cell (SOFC), a chemical process allowing energy to be produced through the transfer of oxide ions between two substrates. Which brings the question of, what can be adjusted? And by how much? Well the SOFC puts this idea into full swing. The present research paper reviews concepts of energy, misfit dislocations in molecular structures, Y-doping and possible material combinations to address this question. Specifically electrolytes within the interface of multiple materials. Leading up to our current field of the study of electrolytes and the instances of misfit dislocations.

The purpose of this paper is to describe and evaluate not only the history relating to SOFC but portray the research of specific material combination our team focused on and additional mathematics to make the process of evaluating misfit dislocations easier.

Introduction

Since the depletion of fossil fuels is now more prominent than ever, new forms of renewable energy must be developed in order to maintain and grow our society. These forms include: solar energy, wind energy, geothermal energy, Hydropower. However there is one in particular that can be extremely resourceful in achieving this mission the Solid Oxide Fuel Cell (SOFC). These cells have the capability to convert chemical energy to electricity. Through taking the porous anode of H2 and transferring oxide ions through an electrolyte into a porous cathode generating electricity while leaving a by-product of H2O. First beginning in 1899, under

the scientist Walter Hermann at the Leipzig's Physicochemical institute. However full focus on this topic wasn't fully focused on until the late 1950s and continues to grow today. With research on multiple parts of SOFC from core technology, system development and cell development. Leading up to the magnitude of material combinations to improve upon this technology. Moreover, it has been found that "Depending on the misfit strain, the interface formed between two materials can be classified into coherent, semi-coherent, or incoherent interfaces. Variance in lattice parameters is mainly responsible for the strain at the in-terface, but the orientation relationship between the two materials is equally culpable for the strain field at the interface." (Pratik P. Dholabhi and Blas P. Ubergauga). Which brings us deeper to the multiple material combinations that can be trialed under this lattice strain to produce the most effective outcome. Additionally, ways of increasing conductivity through the use of Y-doping, as "to ensure high ionic conductivity, oxide materials are generally heavily doped with lower valence elements. This creates a high oxygen vacancy density as a consequence of charge balance....the effect of interfaces on the ionic conductivity of heterostructures composed by an ionic conducting phase and an insulator phase. They investigated the ionic conduction in heterophase boundaries between cubic stabilized zirconia and different insulating oxides, aiming to correlate the interfacial contribution to the multilayer ionic conductivity with the microstructure of the interfaces" (Emiliana Fabbri, Daniel Pergolesi and Enrico Traversa). On top of that, the emissions of SOFC are far less damaging to the environment. Additionally they provide a power output of 100 Watts to 2 MWatts. Along with the massive power output SOFC can be stored relatively easily giving accessibility to power overseas or anywhere without a plug. Yet there is still so much to be developed within this form of energy, specifically the components of the dense electrolyte substrate. Moreover the electrolyte membranes can be manipulated with

different types of materials in order to optimize the energy output without it being too costly or dangerous. Which is why this research holds importance and possibilities.

Methodology

Hypothesis: If a suitable number of columns for new oxides materials are found to work better than others when tested, then it will make SOFCs the future of energy, because efficiency will be increased. This is why new materials need to be tested together computationally so that findings can be passed on and the computational theories relating to the materials can be experimented with the actual materials. We needed to start by looking at how different materials work together.

Our group has looked at different crystalline structures to see where we can optimize and minimize misfit dislocations between both materials. Creating digital combinations of CeO2 at 5.41 A (angstrom) and SrTiO3 at 3.905 A unit cells. As well as BaZrO3 at 4.197 A and MgO at 4.256 A. In order to combine the film and the substrate with the most symmetry therefore mitigating lattice strain we used the equation down below:

$$f = \frac{a_1 - a_2}{a_1}$$

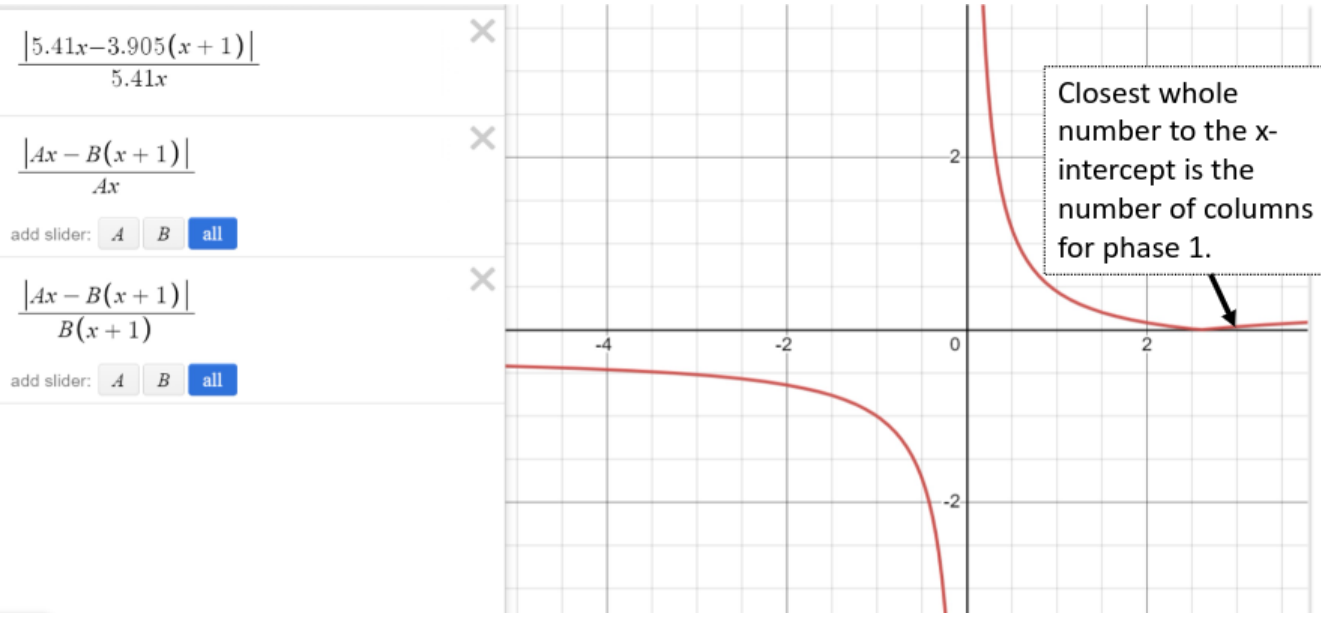
This was the fundamental basis. Where a1 is the lattice parameter of phase 1(film) and a2 (substrate) is the lattice pattern of phase 2. Using this foundation we developed our own equation:

$$f_2 = \frac{|(a_1 \times x) - (a_2 \times (x+1))|}{(a_2 \times (x+1))}$$

This version of the equation is with respect to the substrate, as that is most common. However, it can be with respect to the film as well which would be over a1 x X instead.

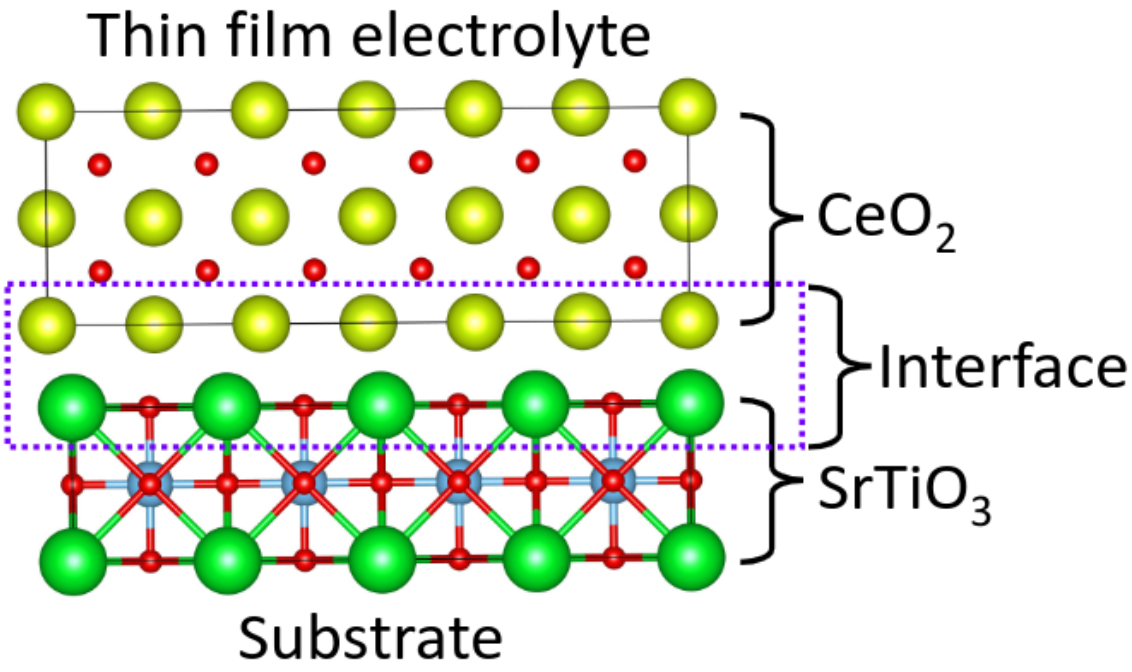
Here, 1 and 2 are lattice parameter of phase 1 (film) and phase 2 (substrate), respectively, while x is constant. is the number of columns for phase 1 and + 1 is the number of columns for phase 2. When this equation is graphed it can be used to calculate the lowest lattice strain with a certain number of columns for any two materials.

The graph below shows the equation being utilized to calculate the lowest lattice strain for SrTiO3 and CeO3:

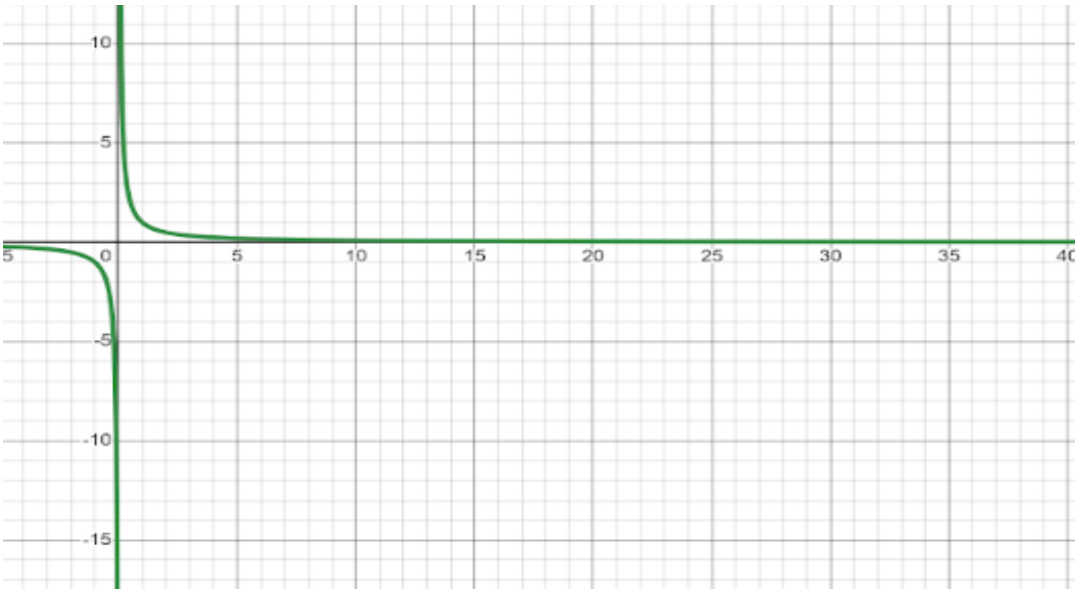


This graph can be interpreted by focusing on quadrant one. As the Y value is equal to the lattice strain, to find the ideal number of columns it's the closest whole number to the x-intercept(where y = 0). This will find the columns for the larger unit cell, then for the smaller unit cell one more column needs to be added. In the above example the x-intercept is closest to three, so the

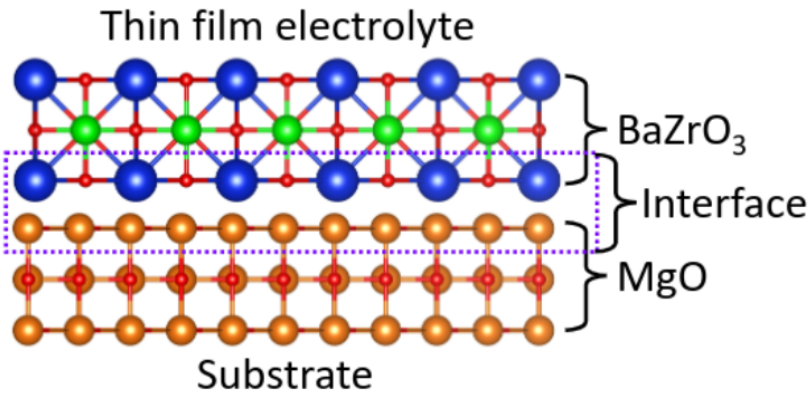
smallest lattice strain will be with three columns of CeO2, and four columns of SrTiO3. This concept is universal and carries on for calculating all column amounts to result in a minimized lattice strain. The original lattice strain for SrTiO3 and CeO2 with just the unit cells is 27.82%. With the three and four columns given by the graph, the lattice strain is 3.76%, showing how much this was minimized by. This allows for the material to line up better at the interface. MgO and BaZrO3 is a molecule that already has a very small lattice strain. This means that MgO and BaZrO3 have very close angstrom amounts in their unit cells, so the misfit dislocation is already minimal as opposed to SrTiO3 and CeO2 which have a greater difference in size of their unit cells, so there's more of a misfit dislocation. However BaZrO3 and MgO lattice strain can still be minimized using our equation. Additionally the image below represents a structure we built of CeO2 with StTiO3. Where the foundation of this structure if produced multiple times will compound the leading up to misfit dislocation.



The graph for finding MgO and BaZrO3 minimum lattice strain is shown below, and it can be observed that the lattice strain doesn't change by much even when the amount of columns change.



Indicating that these materials hold a minimal difference between both interfaces. Resulting in a lattice strain of about 0.04%. Implying that These two materials are able to coexist together in much better conditions compared to other materials. The structure we built computationally of BaZrO3 and Mgo is shown below, these structures were made with a certain amount of columns which we derived from the equation we developed.



Future Works

Right now SOFC's are being studied and experimented with more and more focus, given how beneficial they could be in regards to energy sources. "These developments cause high energy consumption, which leads to the search for clean, secure, affordable and sustainable energy resources."(Singh, Mandeep, 2021) For our specific research, we are planning on continuing to work with different combinations of materials to see how they work relative to what's already been studied. Moreover, seeing how we can optimize electrolytes by-layers in order to minimize lattice strain and maximize energy productivity.

Conclusion

Overall, SOFC holds infinite possibilities for improvement. Where our team has found an easier way to see these possibilities graphically in order to calculate the best options for misfit dislocation between two substances. Making it even more necessary to focus on improving this technology. By eliminating the oxide combination possibilities that are most likely not going to contribute will put this process in the right direction. This specific research is incredibly important currently given that fossil fuels have been depleting for years, and energy replacements that are efficient have to be researched proactively before they run out. Right now it's estimated that oil will run out in 2052, and over the next century coal and gas will be used up as well.(MAHB, 2023). SOFC's are proving to be an efficient and clean alternative and the research being done is already finding ways to improve and discover different oxide combinations so that SOFCs can be an accessible alternative energy source.

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