Theoretical Investigations of the Solid Oxide Fuel Cell Anode

Andres I. Marquez, Yolanda De Abreu, and Gerardine G. Botte

Chemical Engineering Department
Russ College of Engineering and Technology
183 Stocker Center
Ohio University
Athens, OH 45701

Introduction

Several experimental works have been dedicated to understand the behavior of different materials for Solid Oxide Fuel Cells (SOFC), which are becoming very important because: 1. their electrical efficiency is much greater than the one obtained from conventional heat engines and any other type of fuel cells, and 2. they are able to handle some of the contaminants present in syngas, such as CO [1-15]. An extensive review showed that few attempts have been made to use molecular modeling to understand the performance of materials for SOFC applications [16-23]. In the open literature is not reported the use of this technique to aid in the investigation of the interactions of high-temperature anode materials for SOFC with gas-phase components of syngas.

Within this context, the objective of this paper is to model the behavior of the commercial anode materials used in SOFC, Ni-YSZ, in the presence of hydrogen. Computational chemistry techniques such as quantum chemistry (QC) and molecular dynamics (MD) were used for this purpose. Results from the model were compared with experimental data.

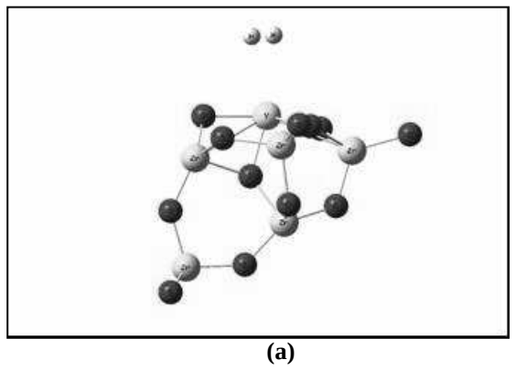
This work should contribute to the development of fuel cell technology, it will create the basis for future modeling and improvement of the performance of anode materials for SOFCs, and should lead to a better understanding of the mechanisms leading to deactivation of the electrode materials.

Methodology

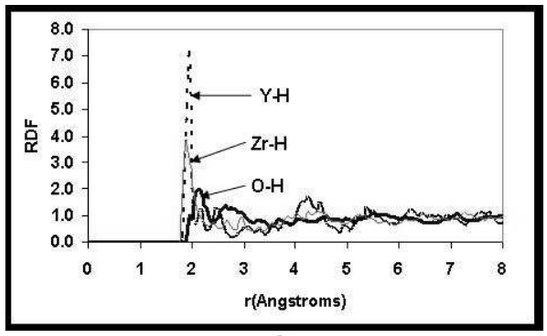
A combination of quantum chemistry (QC) and MD techniques were used to understand the behavior of Ni-Yttrium doped with Zirconia in an H_2 environment. The structures of the molecules involved in the different systems were optimized in gas phase at 0 K and 1 atm at the B3PW91/LANL2DZ level of theory [24]. Gaussian 03 was used for the QC calculations [24]. A frequency analysis of the optimized structures was performed to determine the thermochemistry and to correct the optimized structures and systems for pressure and temperature effects (mainly for the high temperatures found in SOFC operation). The software Cerius2 [25] was used for the MD studies.

Results

Figures 1a and 1b show the interactions of a H_2-YSZ system, having a binding energy of about -12Kcal/mol, which could indicate a strong hydrogen oxidation once it will be compared to others configurations. From MD studies the H atoms interact more strongly with Y atoms of the YSZ. Additional results will be presented and compared to experimental data if available.



(a)



(b)

Fig. 1 (a) Yttria-Stabilized Zirconia cluster model , YSZ (1 Y atom , 5 Zr atoms , 12 O atoms) and H_2; (b) RDFs for YSZ atoms (32 Y, 160 Zr, 384 O) and H_2 (168 H).

References

1. R. Suwanwarangkul et al., J. Po. Sourc., 122, 9 (2003) Solid State Energy Conversion Alliance (SECA), DOE, DE-PS26-04NT42074 Solicitation
2. N. Pujare et al., J. Electrochem. Soc., 134, 2639 (1987).
3. N. Pujare,et al., J. Electrochem. Soc., 136, 3662 (1989).
4. I. Yentekakis and C. Vayenas, JES., 136, 996 (1989).
5. T. Kirk, J. Winnick, J.Electr.. Soc., 140, 3494 (1993).
6. D. Peterson, J. Winnick, JES., 145, 1449 (1998).
7. C. Yates and J. Winnick, JES., 146, 2841 (1999).
8. Y. Matsuzaki , I. Yasuda, Sol. St. Ion., 132, 261 (2000).
9. M. Liu, et al., J. Power Sources, 94, 20 (2001).
10. P. He et al., J. Electrochem. Soc., 149, A808 (2002).
11. M. Liu et al., J. Electrochem. Soc., 150, A1025 (2003).
12. G. L. Wei et al., J. Electro. Soc., 150, A463 (2003).
13. S. Wang et al., J. Sol. St. Electrochem., 5, 188 (2001).
14. L. Zhong, et al., Chinese J. Ch. Engr., 11, 245 (2003).
15. R. Mukundan et al., J. Electroc. Soc., 7, A5 (2004).
16. C. Fisher, H. Matsubara, Sol. S. I., 113, 311 (1998).
17. C. Fisher. H. Matsubara, Co. Mat. S., 14, 177 (1999).
18. C. Fisher, H. Matsubara, J.Eur.Cer. S., 19, 703 (1999).
19. F. Haase, J. Sauer, J.AChem.Soc., 120, 13503 (1998).
20. H. Ogawa, F. Wakai, Mat. Sci. For., 243, 351 (1997).
21. H. Ogawa, F. Wakai, Mat. Sci. For., 357, 571 (2001).
22. H. Ogawa, F. Wakai, Mat. Trans., 42, 2266 (2001).
23. F. Wakai, et al., Mater. Character., 37, 331 (1996)
24. E. Frisch and M.J. Frisch, Gaussian 03 User's Reference, Gaussian Inc., Pittsburgh (2003).
25. Accelrys, Cerius2, Accelrys, San Diego, CA (2003).