Mixed Ionic and Electronic Conduction of Y-Doped BaZrO\textsubscript{3}

Wensheng Wang and Anil V. Virkar\textsuperscript{1}

Department of Materials Science & Engineering
122S Central Campus Drive, University of Utah
Salt Lake City, UT 84112
Email: anil.virkar@m.cc.utah.edu

INTRODUCTION

Rare earth-doped BaZrO\textsubscript{3} ceramics contain oxygen vacancies and can exhibit substantial proton conduction in humid atmospheres at elevated temperatures \[1\]. Of the many rare-doped BaZrO\textsubscript{3} materials, Y-doped BaZrO\textsubscript{3} combines high proton conductivity and excellent stability in CO\textsubscript{2} and H\textsubscript{2}O containing atmospheres, which makes it a promising electrolyte material for use in solid-state electrochemical devices \[2\]. It is therefore important to study electrical conductivity under various conditions of practical interest. Previous studies suggest that Y-doped BaZrO\textsubscript{3} can exhibit predominantly electron-hole conduction or ionic conduction, depending on the partial pressure of oxygen \[3\]. However, the relative magnitudes of conductivities due to oxygen ion, proton, and electron-hole are yet not clear. This work reports on our recent studies on mixed conduction of Y-doped BaZrO\textsubscript{3} over a wide range of O\textsubscript{2}, H\textsubscript{2}O, and temperature.

EXPERIMENTAL

Y-doped barium zirconate of composition BaZr\textsubscript{0.93}Y\textsubscript{0.07}O\textsubscript{3-δ} was synthesized using a conventional solid-state method. Bar-shaped porous samples with ~40 vol.% porosity were made by adding fine carbon beads followed by sintering. Platinum paste was painted on the sample surface, followed by firing at 900°C for three hours to produce reliable electrical contacts. Resistance measurements were made using a 4-probe dc technique at several temperatures and under various partial pressures of O\textsubscript{2} and H\textsubscript{2}O. Water vapor was supplied by passing the carrier gas through a water bubbler at the desired temperature.

RESULTS AND DISCUSSION

Electrical conductivity was first measured in humidity-free atmospheres at various p\textsubscript{O\textsubscript{2}} levels over a temperature range from 500 to 800°C, as shown in Fig. 1. The conductivity is proportional to p\textsuperscript{-1/4} for p\textsubscript{O\textsubscript{2}} <0.1 atm. at 500°C, indicative of electron-hole conduction. By fitting the data to the expression \[\sigma = A + Bp_{O_2}^{\alpha}\], values for \(A\) and \(B\) were determined for each of the four temperatures. The temperature dependence of \(B\) yields an estimate of the activation energy for electron-hole conduction, which is 0.99 eV, as shown in Fig. 2.

The p\textsubscript{H\textsubscript{2}O} -dependence of electrical conductivity was also investigated at various p\textsubscript{O\textsubscript{2}} and various temperatures. At p\textsubscript{O\textsubscript{2}} of 0.2 atm and with increasing p\textsubscript{H\textsubscript{2}O}, the measured total conductivity increases at 500°C but decreases at 700°C. At p\textsubscript{O\textsubscript{2}} of ~0.0015 atm, however, the conductivity increases at 500 and 700°C with increasing p\textsubscript{H\textsubscript{2}O}. Further data analysis concerning the conductivities due to three charge species and their dependence on p\textsubscript{O\textsubscript{2}}, p\textsubscript{H\textsubscript{2}O}, and temperature will be presented.

ACKNOWLEDGEMENTS

This work is supported by the U.S. Department of Energy, under grants DEFG0397ER45661 and DEFG0203ER46086

REFERENCES


1 To whom correspondence should be addressed