Solutions (approximately) to theHW Exam on Electrochemistry

1: Narrative on Comparing SOFCs and Li-ion Batteries

Write less than on page to compare the similarities and differences between a Solid Oxide Fuel Cell and a battery such as the lithium-ion batteries.

The two system have a lot in common, in terms of having an anode (oxidation), electrolyte (ion conductor), and a cathode (reduction).

The main difference is that SOFC run on fuel, like a car, while batteries store charge in the anode, which is transferred to the cathode as the battery discharges, and back to the anode during recharge. Therefore the functions of the anode and cathode are different, and therefore the basis for selecting the materials for them is very different for the SOFCs and the lithium ion battery. In the battery the chemical potential of the Li in the electrodes determines the cell voltage. In an SOFC the ratio of the partial pressure of oxygen (at the cathode and the anode) determines the cell voltage.

2. ASR

Give reasons why ASR (area specific resistance) has units of Ωcm^2 and not Ωcm^{-2}.

ASR is used to calculate the cell voltage from the current density. The Nernst Potential, Cell voltage and the current density are the three fundamental performance parameters for SOFCs and for batteries.

The cell voltage = Nernst voltage - (voltage drop across the cell)

The voltage drop across the cell = current density * ASR. Therefore ASR must have units of Ohm cm^2.

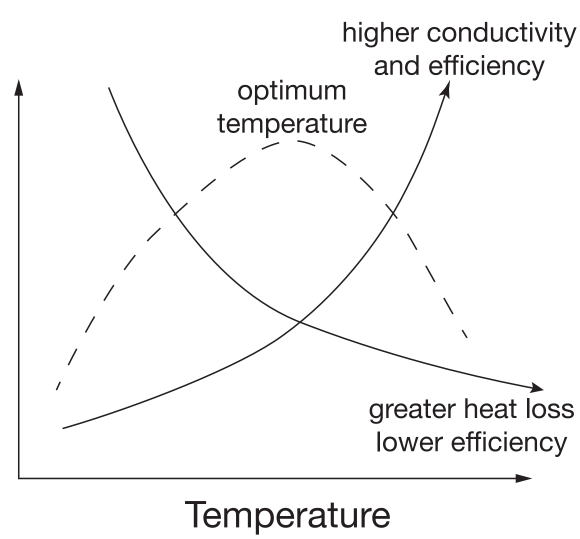
3. Temperature for SOFC Operation

Why does an SOFC be operated at elevated temperature?

Can you draw a sketch of competing parameters that lead to an optimum temperature for cell operation? (The term competing means that one increases the efficiency of the fuel cell while the other reduces the overall efficiency of the system)

The cell efficiency depends on the ionic conductivity of the electrolyte. The higher the conductivity the better. The ionic conductivity is related to the diffusion coefficient of the "ion". High temperature of the SOFC increases the ionic conductivity.

However, high operating temperature requires heating which is an energy cost. As shown below the juxtaposition of these two effects means that optimum conditions are obtained at an intermediate temperature, since the overall efficiency is the product of these two "efficiencies".



4. Power Delivery from SOFCs

Explain, with elementary sketches and equations if you wish, why the curve for the power density vs. current density shows a maximum. (From my point of view the best answer would be if you can explain with words alone - with physical arguments).

Power delivery is the product of the cell voltage and the current. The cell voltage is equal to the difference between the Nernst voltage (at zero current) and the internal drop in the voltage due to the intrinsic resistance of the cell. The voltage drop increases as the current increases. If one takes the limits at zero current and at very large current, then one finds that both extremes give zero power: at zero current and the Nernst potential the power is zero because the current is zero. At very high current the internal voltage drop can become equal to the Nernst potential so that the cell voltage begins to approach zero, again the power delivered approaches zero. Between these two limits that has to be a maximum.

5. Electrolyte Chemistry for SOFCs

Explain why yttria doped zirconia is the material of choice as the electrolyte for SOFCs.

The oxygen ion conductivity is enhanced by oxygen vacancies. The replacement of ZrO_2 or Zr_2O_4 by Y_2O_3 leaves on oxygen site vacant, hence oxygen ion diffusion is enhanced.

6. Architecture of Li-ion batteries

Why are Li-ion batteries constructed from three layers - the anode, the electrolyte and the cathode. What are the functions of these three elements and what properties will you use for selecting the appropriate materials for them?

The battery must have a difference in the chemical potential between the anode and the cathode to generate a voltage. The electrolyte separating the electrodes seeks to transport lithium ions from the high chemical potential(anode) to the low chemical potential (cathode).

7. The Performance Parameters (units)

Give the units for the following

Charge capacity of the anode?

mAh/g

Energy density of a battery?

kWh/kg, or kWh/m^3, the first is the gravimetric and the second the volumetric energy density.

Capacity per unit area of the battery?

mAh/cm^2

8. Overall Performance Parameters

Derive an equation that relate the gravimetric capacity of the battery to the charge capacity of the anode (assume that the weight of the anode constitutes one third of the total weight of the battery).

The charge capacity of the anode has units of mAh/g; Leg us say it is $\overline{C}_A$ mAh/g, then the charge capacity expressed in terms of the total wt of the battery will be

$\overline{C}_B = \frac{1}{3}\overline{C}_A$ mAh/g; this is now the gravimetric capacity of the battery. It can be converted into Coulombs/g by dividing by 1000 (to convert mA into A) and dividing again by 3600 to convert h into seconds.

9. Lithium Metal Anodes

Derive the capacity of lithium metal anodes from first principles in units of mAh g^{-1}.

One lithium atom can provide a charge of one electron. Therefore one mole of Li metal can provide a charge of one Faraday, that is, 96500 Coulombs, or 96500 As (ampere seconds), or (96500/3600)=28.6 Ah, or 28.6*1000 mAh/mol of Li metal.

One mole of lithium metal weighs 6.94 g/mol (i.e.mol wt of Li)

Therefore the capacity of Li metal is 28.6*1000/6.94 mAh/g = 4121 mAh/g

10. Building a Car Battery

•Explain why the specifications for EV-cars are given in terms of kWh.

•Look up the capacity and voltage of the battery in your own computer, and calculate how many such batteries would be need to create a 75 kWh battery for a car.

kWh is the total energy that a battery can deliver; it can therefore be related to how far the car can be driven with one charge. It is like miles per gallon for IC engines.

My computer has an about 12 V battery (actually 11.4 volt) battery with a maxium charge capacity of 7828 mAh, so that it can deliver (7828/1000)*12 Wh, or 12*7.828/1000 kWh of energy. Thus about 800 computer batteries would equal a 75 kWh car battery.