Empirical equation about open circuit voltage in SOFC

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Using doped Ceria electrolytes or doped Bismuth electrolytes in SOFCs, the V_{oc} (open circuit voltage) become lower than the Nernst voltage which are got from using YSZ (Yttria stabilized Zirconia) electrolytes. Empirical equations about these open circuit voltage in SOFCs are presented in this letter.

1. Empirical equation about the V_{oc} (open circuit voltage)

When the t_{ion} (ionic transference number) is almost unity at the cathode side and t_{ion} is small enough at the anode side, the new equation for the V_{oc} is expressed as:

$$V_{oc} = V_{th} - E_a/2e. \quad (1)$$

E_a is the activation energy of the oxygen ions. Vth is Nernst voltage.

There are many reports which give the data of doped Ceria electrolytes (e.g. [1]) and they are presented in Table I. The data for the activation energy of doped Bismuth is from [2]. In [2], activation energy is 1.0 eV (=100 kJ/mol = 30 kJ/mol + 70 kJ/mol). About the open circuit voltage of doped Bismuth electrolytes, this material is too weak under reducing atmosphere to measure in safety. But the value of the open circuit voltage is known to be about 0.6–0.7 V.

As shown in Table I, the predictions from the empirical Equation 1 is good match with experimental results for these materials.

2. Generalized empirical equation about the V_{oc}

When the t_{ion} is unity at the cathode side, the new equation for the V_{oc} is expressed as:

$$V_{oc} = V_{th} - (1 - t_{ion}) \times \frac{E_a}{2e} \quad (2)$$

TABLE I Example of empirical equation (Vth is 1.15 V around 1073 K)

Material	V_{oc} (V)	E_a (eV)	Calculated V_{oc}
Sm_2O_3 doped CeO_2	0.81	0.68	0.81 V = 1.15 − 0.68/2
Gd_2O_3 doped CeO_2	0.78	0.74	0.78 V = 1.15 − 0.74/2
CaO doped CeO_2	0.74	0.83	0.74 V = 1.15 − 0.74/3
Er_2O_3 doped Bi_2O_3	0.6–0.7	About 1.0	0.65 V = 1.15 − 1.0/2

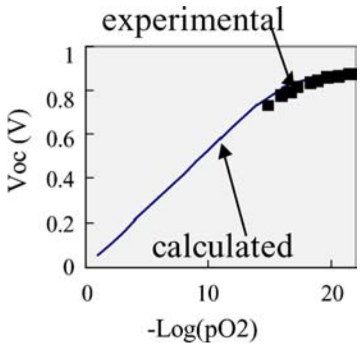

Figure 1 PO_2–V_{oc} characteristic.

This t_{ion} is the ionic transference number near the anode surface which can be calculated using temperature and the anode oxygen gas pressure.

For example, for doped Ceria t_{ion} [3]:

$$t_{ion} = 1/[1 + (PO_2/PO_2^*)^{-1/4}] \quad (3)$$

PO_2 is the pressure of oxygen on the anode side. $PO_2{}^*$ is constant and is the pressure of oxygen where t_{ion} equals to 0.5. The real line is calculated by Equation 2 when $PO_2{}^*$ is 5×10^{-20} atm and $E\alpha$ is 0.68 eV. The square black symbols are experimental results at 750 °C on doped CeO_2 [4].

Fig. 1 demonstrates the curve of empirical Equation 2 is good match for the experimental data.

References

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