In-Class Exercise
Perovskite Structure
SOLUTION

Calculate the IPF (ionic packing factor) in perovskite. What do you think would happen if the materials were produced without porosity in an SOFC? Could there be atom transport across?

In order to calculate the density, we need to know the volume of the unit cell. For this, we need the atomic radii:

$r_{Mn^{3+}} = 0.785$ Å – This ionic radius corresponds to a coordination number of [6]*

Reference: D.W. Richerson, Modern Ceramic Engineering 2/e, (Marcel Dekker, New York, 1992), pg. 845.

$r_{La^{3+}} = 1.320$ Å – This ionic radius corresponds to a coordination number of [12]

Reference: D.R. Lide, CRC Handbook of Chemistry and Physics 71/e, (CRC Press, Boca Raton, 1990), pg. 4-126.

$r_{O^{2-}} = 1.28$ Å – This ionic radius corresponds to a coordination number of [8]

Reference: D.W. Richerson, Modern Ceramic Engineering 2/e, (Marcel Dekker, New York, 1992), pg. 846.

Since the atoms are in contact along the face diagonal, the following relationship applies:

$$2r_{La^{3+}} + 2r_{O^{2-}} = a\sqrt{2}$$

We can then solve for the lattice parameter:

$$a = \frac{2r_{La^{3+}} + 2r_{O^{2-}}}{\sqrt{2}} = \frac{2\cdot(1.320)+2\cdot(1.28)}{\sqrt{2}} = 3.68 \text{ Å}$$

Since the unit cell is a cube, the volume is:

$V_c = a^3 = (3.68 \text{ Å})^3 = 49.7 \text{ Å}^3 (1 \times 10^{-10} \text{ m/Å})^3 = 4.97 \times 10^{-29} \text{ m}^3$

The atomic (ionic) packing factor for this structure is:

$$IPF = \frac{V_{atoms}}{V_c} = \frac{\frac{4}{3}\pi r_{Mn^{3+}}^3 + \frac{4}{3}\pi r_{La^{3+}}^3 + 3\cdot\frac{4}{3}\pi r_{O^{2-}}^3}{V_c}$$

$$IPF = \frac{\frac{4}{3}\pi(0.785)^3 + \frac{4}{3}\pi(1.320)^3 + 3\cdot\frac{4}{3}\pi(1.28)^3}{49.7} = \frac{38.0}{49.7} = 0.765$$

This is a very tight arrangement of atoms. Since there is little empty space between the atoms, if the cathode in the SOFC was prepared without pores, the oxygen could not be transported into the electrolyte in an efficient manner.