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APPENDICES

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

APPENDIX A

The Calculation of Tolerance Number

Goldschmidt (1926) defined the tolerance limits of the size of ions through a tolerance factor, t as Equation (A.1)

$$t = (r_A + r_O) / [\sqrt{2} (r_B + r_O)] \quad (\text{A.1})$$

where r_A , r_B , and r_O are the radii of respective ions. For the substituted perovskite at A and B site, $A_{1-x}A'_x B_{1-y}B'_y O_{3-\delta}$, r_A and r_B were calculated from the sum of each metal at A site and B site, respectively, time its composition. The atomic weight, ionic charge, coordination number, and ionic radius of all concerned metals were shown in Table A.1

Table A.1 Atomic weight, ionic charge, coordination number, and ionic radius of concerned metals

Metal	Atomic weight	ionic charge	Coordination No.	ionic radius (Å)
La	138.92	3+	12	1.36
Fe	55.85	3+	6	0.55
Ga	69.72	3+	6	0.62
Ba	137.36	2+	12	1.61
Sr	87.62	2+	12	1.44
Co	58.94	2+	6	0.65
O	16.00	2-	6	1.40

Therefore, as Equation A.1 the tolerance number of perovskite compounds such as LSGF6428 was calculated as below.

$$\begin{aligned} \text{tolerance number of LSGF6428} &= \frac{1.36*0.6+1.44*0.4+1.40}{\sqrt{2} (0.55*0.8+0.62*0.2+1.40)} \\ &= 1.01 \end{aligned}$$

APPENDIX B

The Calculation of the Oxygen-Permeation Rate

The oxygen-permeation rates for perovskite membranes were measured by gas chromatography with helium as a carrier gas. Gas standards were made by varying the oxygen concentration in helium. The formulas for calculating oxygen permeation rates are presented as follows:

$$J(\text{cm}^3(\text{STP})/\text{min}/\text{cm}^2) = v_{s,\text{He}}(T_s, P_s) \times R(\text{O}_2/\text{He})/S \quad (\text{B.1})$$

Where $v_{s,\text{He}}(T_s, P_s)$ ($\text{cm}^3(\text{STP})/\text{min}$) is the volumetric flow rate of pure helium at the standard state condition, $R(\text{O}_2/\text{He})$ is the ratio of the oxygen volumetric fraction to the helium volumetric fraction, and S is the oxygen permeation area, 0.283 cm^2 . The permeation rate J ($\text{cm}^3(\text{STP})/\text{min}/\text{cm}^2$) multiplied by the factor of 7.4358×10^{-7} can be transferred to another unit ($\text{gmol}/\text{s}/\text{cm}^2$).

The $v_{s,\text{He}}(T_s, P_s)$ is calculated from the slope of mass-controller calibration line for helium, which is calibrated by a bubble flowmeter, as in Figure B.1, and the slope of oxygen calibration line, as in Figure B.2. The equation for calculation the $v_{s,\text{He}}(T_s, P_s)$ is shown in Equation 2

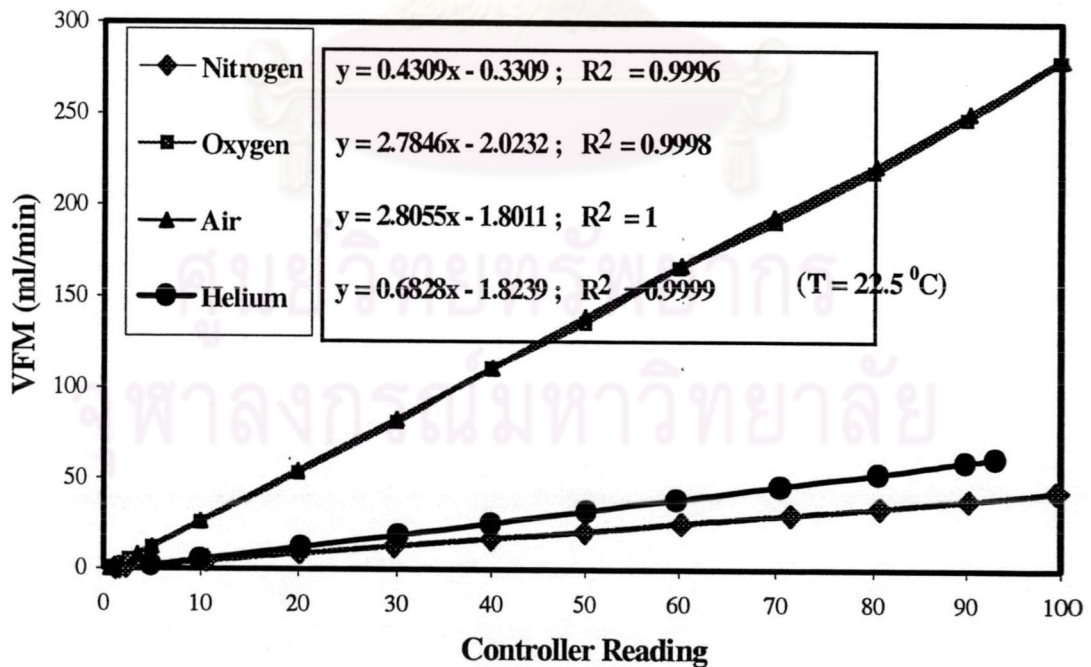


Figure B.1 Mass-controller calibration line for nitrogen, oxygen, air, and helium

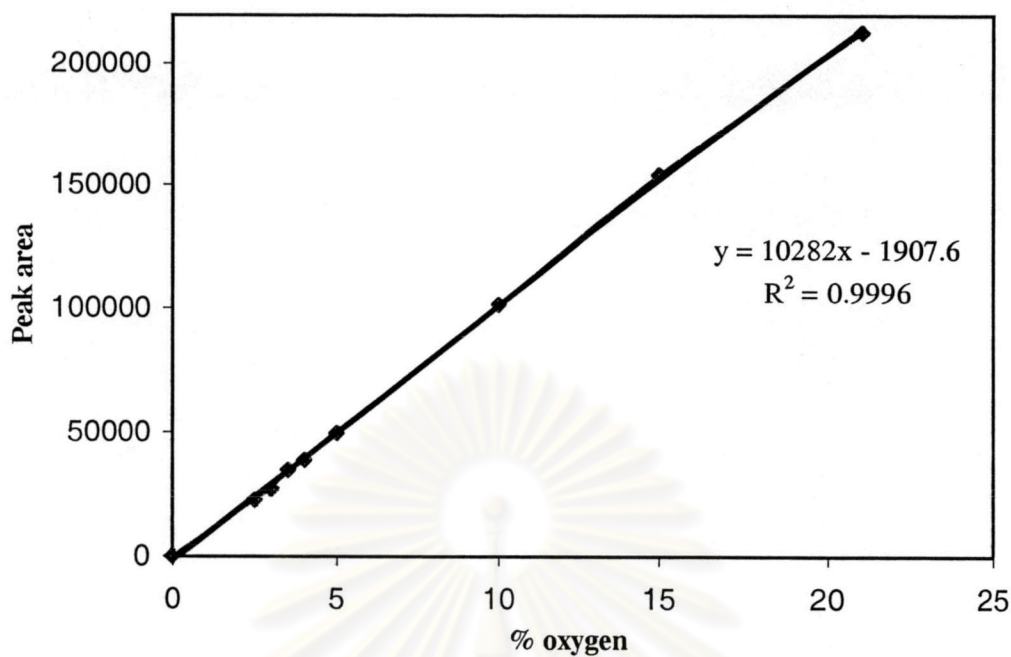


Figure B.2 Oxygen Calibration curve

$$v_{s,He}(T_s, P_s) = \text{Readings} \times 0.6828 \times P_c/T_c \times T_s/P_s \quad (\text{B.2})$$

$$R(\text{O}_2/\text{He}) = \text{area of O}_2 / (10282 - \text{area of O}_2) \quad (\text{B.3})$$

Where P_c , T_c = ambient pressure and temperature, respectively, P_s , T_s = pressure and temperature at the standard state (760 mmHg), 273.15 K), respectively. The final equation for J is as follows:

$$J = \text{Reading} \times 0.6828 \times P_c/T_c \times T_s/P_s \times R(\text{O}_2/\text{He}) / S \quad (\text{B.4})$$

APPENDIX C

Raw Data from the XRD Pattern of $\text{La}_{0.6}\text{Sr}_{0.4}\text{Ga}_{0.8}\text{Fe}_{0.2}\text{O}_{3.5}$

In the general basic, the crystal structure of a substance determines the diffraction pattern of that substance or, more specifically, that the shape and size of the unit cell determines the angular positions of the diffraction lines, and the arrangement of the atoms within the unit cell determines the relative intensities of the lines. Since the structure determines the diffraction patterns, the raw data of crystal structure can be obtained from the XRD pattern. In Figure C.1, the XRD pattern shows the raw data of the spacing d , 2-Theta, and peak intensity of any particular set of lattice planes (hkl).

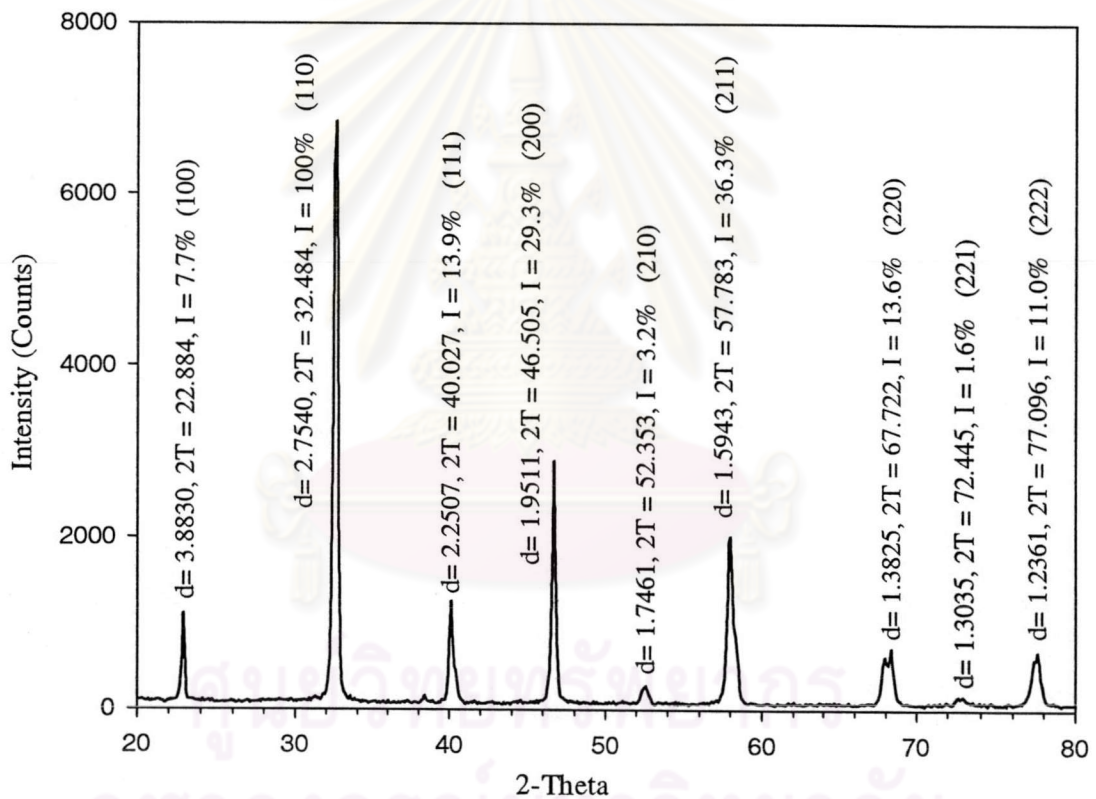


Figure C.1 XRD Pattern of $\text{La}_{0.6}\text{Sr}_{0.4}\text{Ga}_{0.8}\text{Fe}_{0.2}\text{O}_{3.5}$

These raw data can be used to calculate the lattice parameter as shown in Appendix D.

APPENDIX D

The Calculation of the Theoretical Density

The theoretical density is calculated from the theoretical weight (W_t), which is from the molecular formula of $La_{0.6}Sr_{0.4}Ga_{0.2}Fe_{0.8}O_{3-\delta}$, and the theoretical volume (V_t), which is calculated from the lattice parameter, as in Equation 1

$$D_t = W_t / V_t \quad (D.1)$$

$$V_t = a^3 \quad (D.2)$$

The non-stoichiometry of oxygen in mole formula, δ , is calculated from the difference of the total charge of oxygen and metals divided by charge of oxygen.

For example, W_t of $La_{0.6}Sr_{0.4}Ga_{0.2}Fe_{0.8}O_{3-\delta}$, is

$$\begin{aligned} &= 138.92 \times 0.6 + 87.62 \times 0.4 + 69.72 \times 0.2 + 55.85 \times 0.8 + \\ &\quad 16 \times \{3 - \{6 - (3 \times 0.6 + 2 \times 0.4 + 3 \times 0.8 + 3 \times 0.2)\} / 2\} \\ &= 221.804 \text{ g/mol} \\ &= 36.84 \times 10^{-23} \text{ g/molecule} \end{aligned}$$

For the cubic system, lattice parameters (a) are calculated from Bragg's Equation, as in Equation (D.3), and the plane spacing equation, as in Equation (D.4).

$$\lambda = 2d \sin \Theta \quad (D.3)$$

$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)}{a^2} \quad (D.4)$$

where λ is the wavelength of X-ray beam, d is the distance between adjacent planes in the set (hkl), and 2Θ is the diffraction angle.

Therefore, the lattice parameter equation is shown in Equation (D.5)

$$a = \sqrt{d^2 \times (h^2 + k^2 + l^2)} \quad (D.5)$$

As the XRD pattern of LSGF6428 in Appendix C, all the possible Bragg angles at which diffraction can occur form the reflective planes of 100, 110, 111, 200, 210, 211, and 220. The parameter a is directly proportional to the spacing d of any particular

set of lattice planes. Thus the precise parameter method is required and involved the following Equation:

$$a = a_0 + a_0K\cos^2\Theta = a_0 + a_0K(1-\sin^2\Theta) \quad (D.6)$$

Hence, for cubic substances, if the value of a computed for each line on the pattern is plotted against $\cos^2\Theta$, a straight line should result, and a_0 , the true value of a , can be found by extrapolating this line to $\cos^2\Theta = 0$. Since $\sin^2\Theta = 1 - \cos^2\Theta$, the various values of a may be plotted against $\sin^2\Theta$, and the line extrapolated to $\sin^2\Theta = 1$. In Figure D.1, these values of a from XRD pattern in Appendix C are plotted against $\sin^2\Theta$, and a_0 is found by extrapolation to be 3.912 Å.

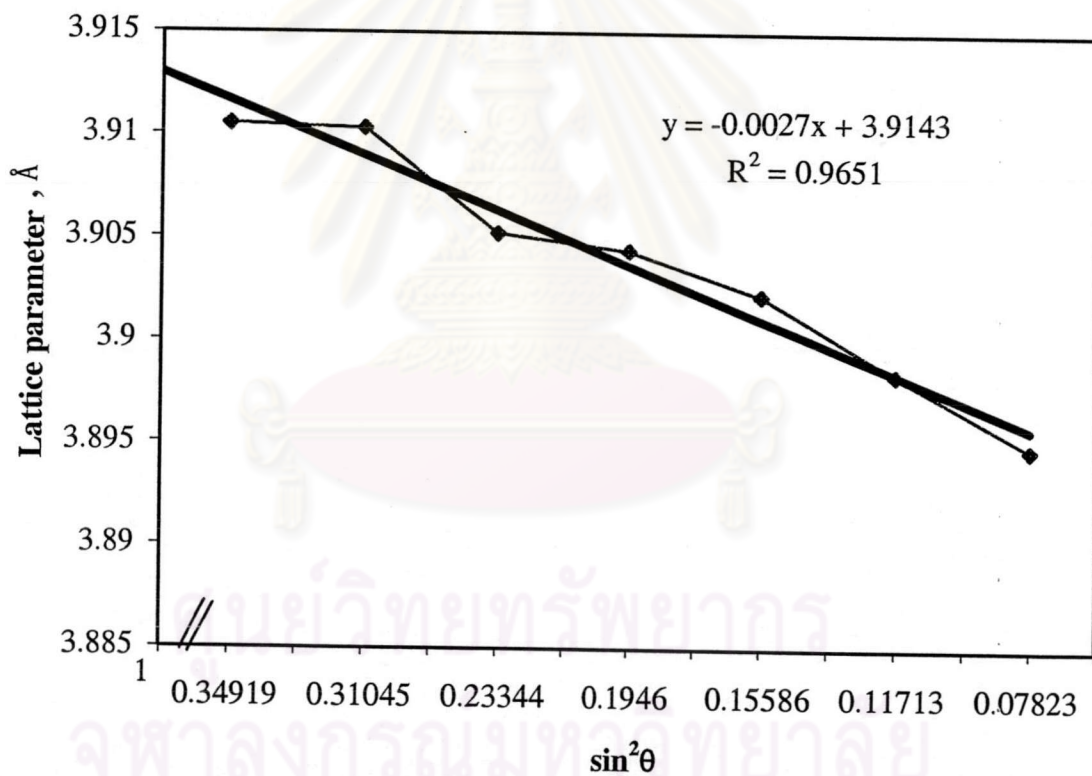


Figure D.1 Extrapolation of measured lattice parameters against $\sin^2\Theta$

When substituted W_t , and a_0 in Equation D.1, therefore, the theoretical density of LSGF6428 is

$$\begin{aligned} &= \frac{36.8 \times 10^{-23} \text{ g/molecule}}{(3.912 \times 10^{-8} \text{ cm})^3} \\ &= 6.15 \text{ g/cm}^3 \end{aligned}$$

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