

How to Calculate Binary Metal Oxyhydroxide Film Catalysts ?

如何定義與計算二元金屬薄膜氫氧化物 ?

動機 (Motivation)

本實驗室催化劑皆以薄膜形式生長，厚度薄且重量極輕。因此天秤難以衡量，所以想另找方式得知負載量。 All of catalysts grown by form of film in this lab, it has thin thickness and lightest weight. Therefore, it difficultly measure loading by precision balance, so need to find another way to know.

原始數據 (Raw Data)

最後可透過ICP-MS的分析數據，以CMOH為例。加上張仁懷學長推導CMOH薄膜沉積反應式，計算各元素的毫莫耳數與負載量後，加總即可得知該催化劑之負載量。

Final, would like to through analytical data by ICP-MS, take CMOH film catalyst for example. Base on the deposition equation of CMOH film that Jhang Ren-Huai had already derivate, after calculating the mmol and loading of various elements, summed up those results to know loading of CMOH film.

CMOH-1					CMOH-2				
4	原始數據	上機稀釋倍數	實際濃度(ppm)	RSD (%)	7	原始數據	上機稀釋倍數	實際濃度(ppm)	RSD (%)
Co (mg/L)	1.789	3	5.367	0.68%	Co (mg/L)	2.026	3	6.078	0.57%
Fe (mg/L)	ND(<0.05 ppm)	3	ND(<0.15 ppm)		Fe (mg/L)	ND(<0.05 ppm)	3	ND(<0.15 ppm)	
Mn (mg/L)	0.574	3	1.723	0.59%	Mn (mg/L)	0.640	3	1.919	0.57%
CMOH-3					CMOH-4				
8	原始數據	上機稀釋倍數	實際濃度(ppm)	RSD (%)	6	原始數據	上機稀釋倍數	實際濃度(ppm)	RSD (%)
Co (mg/L)	1.924	3	5.772	0.09%	Co (mg/L)	1.766	3	5.298	0.16%
Fe (mg/L)	ND(<0.05 ppm)	3	ND(<0.15 ppm)		Fe (mg/L)	ND(<0.05 ppm)	3	ND(<0.15 ppm)	
Mn (mg/L)	0.612	3	1.835	0.12%	Mn (mg/L)	0.573	3	1.718	0.11%

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Step 1. 計算鈷錳元素的毫莫耳數，但由於委測樣品溶液為10毫升，因此需做校正。

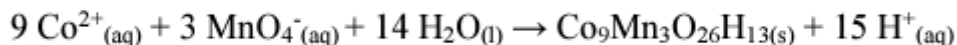
In step 1, calculate the mmol of cobalt and manganese content. But due to commissioned sample solution was given 10 mL to NCKU, so need to calibrate equation.

$$Co\text{ mmol} = \frac{Weight}{M.W.} = \frac{5.367\text{ (mg/L)} \times 0.01\text{ (L)}}{58.9} = 9.253 \times 10^{-4}$$

$$Mn\text{ mmol} = \frac{Weight}{M.W.} = \frac{1.723\text{ (mg/L)} \times 0.01\text{ (L)}}{54.9} = 3.138 \times 10^{-4}$$

Step 2. 使用CMOH薄膜沉積反應式中的催化劑化學式，並以鈷元素的毫莫耳數作為定值，利用元素比例推算各元素之數值。

Using catalyst chemical formula which in the deposition equation of CMOH film, and then take the mmol of cobalt be a constant value, Estimating the value of various elements by formula ratio.



$$O\text{ mmol} : \frac{26 \times Co\text{ mmol}}{9} = \frac{26 \times 9.253 \times 10^{-4}}{9} = 2.673 \times 10^{-3}$$

$$H\text{ mmol} : \frac{13 \times Co\text{ mmol}}{9} = \frac{13 \times 9.253 \times 10^{-4}}{9} = 1.336 \times 10^{-3}$$

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Step 3. 假設當以錳元素的毫莫耳數作為定值時，利用元素比例推算各元素之數值。

Assume when constant value change to the mmol of manganese, Estimating the value of various elements by formula ratio.

$$O \text{ mmol} : \frac{26 \times Co \text{ mmol}}{3} = \frac{26 \times 9.253 \times 10^{-4}}{3} = 2.720 \times 10^{-3}$$

$$H \text{ mmol} : \frac{13 \times Co \text{ mmol}}{3} = \frac{13 \times 9.253 \times 10^{-4}}{3} = 1.360 \times 10^{-3}$$

Step 4. 得知各元素之毫莫耳數後，分別乘於該元素之原子量即可得到其重量，並計算總合作為催化劑的整體負載量。

After knowing each mmol of elements, multiplying by atomic weight of each elements that you can get loading weight, respectively. And then added up each weight to be overall loading of the catalyst.

$$Co \text{ loading (mg/cm}^2\text{)} : Co \text{ mmol} \times 58.9332 = 9.253 \times 10^{-4} \times 58.9332 = 0.054533532$$

$$Mn \text{ loading (mg/cm}^2\text{)} : 3.138 \times 10^{-4} \times 54.938 = 0.017241926$$

$$O \text{ loading (mg/cm}^2\text{)} : 2.673 \times 10^{-3} \times 15.999 = 0.042768821$$

$$H \text{ mmol (mg/cm}^2\text{)} : 1.336 \times 10^{-3} \times 1.0078 = 0.001347035$$

$$Total \text{ loading (mg/cm}^2\text{)} : Loading_{Co+Mn+O+H} = 0.115891314$$

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Step 5. 因負載量由不同定值進行計算，為了避免尷尬的問題，所以將兩種計算結果進行平均後，可得二元金屬薄膜氫氧化物之負載量。

Because calculate the total loading by constant value of cobalt or manganese, to avoid embarrassing issues, so two different results will be averaged to get the average loading of binary metal oxyhydroxide film catalyst.

$$\text{Average loading : } \frac{\text{Total loading}_{\text{Co}} + \text{Total loading}_{\text{Mn}}}{2} = \frac{0.115891314 + 0.116662945}{2}$$
$$= 0.116277129$$

Step 6. 由於寄送ICP-MS樣品為1 cm × 1 cm尺寸的CMOH GDE，因此最終數值不需再除以面積，即可得mg/cm²。

Due to sent ICP-MS samples by cutting 1 cm × 1 cm from 5 cm × 5 cm CMOH GDE, therefore the final result didn't divide by the size area of GDE, can directly get mg/cm².

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不同CMOH 薄膜催化劑之負載量(the average loading of different trials of CMOH film)

表 1 透過 ICP-MS 計算不同 CMOH 薄膜催化劑之負載量

Entry	1	2	3	4
Trials	CMOH-1	CMOH-2	CMOH-3	CMOH-4
^a Real Conc.	5.367 (Co)	6.078 (Co)	5.772 (Co)	5.298 (Co)
(ppm)	1.723 (Mn)	1.919 (Mn)	1.835 (Mn)	1.718 (Mn)
Co (mmol)	9.253×10^{-4}	1.048×10^{-3}	9.952×10^{-4}	9.134×10^{-4}
Mn (mmol)	3.138×10^{-4}	3.495×10^{-4}	3.342×10^{-4}	3.129×10^{-4}
O (mmol)	^b 2.673×10^{-3}	^b 3.027×10^{-3}	^b 2.875×10^{-3}	^b 2.639×10^{-3}
	^c 2.720×10^{-3}	^c 3.029×10^{-3}	^c 2.899×10^{-3}	^c 2.712×10^{-3}
H (mmol)	^b 1.336×10^{-3}	^b 1.514×10^{-3}	^b 1.437×10^{-3}	^b 1.319×10^{-3}
	^c 1.360×10^{-3}	^c 1.515×10^{-3}	^c 1.448×10^{-3}	^c 1.356×10^{-3}
Total Loading	^b 0.115891314	^b 0.130921371	^b 0.124456285	^b 0.114573009
(mg/cm ²)	^c 0.116662945	^c 0.130954879	^c 0.1248167	^c 0.115781549
Ave. Loading	0.116277129	0.130938125	0.124636493	0.115177279
(mg/cm ²)				

a. : Real concentration of Co and Mn element came from row datas by ICP-MS ; b. : The mmol of elements and total loading calculated from the mmol of cobalt as fixed value ; c. : The mmol of elements and total loading calculated from the mmol of manganese as fixed value