

Appendix B

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Error Analysis

B.1 Refractive Index $[n(\lambda)]$

$$n(\lambda) = \left[N + (N^2 - n_0 n_1)^{\frac{1}{2}} \right]^{\frac{1}{2}}$$

where;

$$N(\lambda) = \frac{n_0^2 + n_1^2}{2} + 2n_0 n_1 \frac{T_{\max}(\lambda) + T_{\min}(\lambda)}{T_{\max}(\lambda) T_{\min}(\lambda)}$$

$$\left[\frac{\Delta T_{\max}}{T_{\max}} \right] = \left[\frac{\Delta T_{\min}}{T_{\min}} \right] \approx 10^{-2}$$

$$\left[\frac{\Delta N(\lambda)}{N(\lambda)} \right]^2 = \left[\frac{\Delta T_{\max} + \Delta T_{\min}}{T_{\min}} \right]^2 + \left[\frac{\Delta T_{\max}}{T_{\max}} \right]^2 + \left[\frac{\Delta T_{\min}}{T_{\min}} \right]^2$$

$$\left[\frac{\Delta N(\lambda)}{N(\lambda)} \right]^2 = 2.806 \times 10^{-3}$$

$$\left[\frac{\Delta N(\lambda)}{N(\lambda)} \right]^2 = \left[\frac{\Delta n(\lambda)}{n(\lambda)} \right]^2 = 2.806 \times 10^{-3}$$

$$\left[\frac{\Delta n}{n} \right] = 0.05$$

B.2 Thickness

$$\Delta d = \sqrt{\frac{\sum (d - d^i)}{N(N-1)}}$$

$$\Delta d = \pm 6.0$$

B. 3 Hydrogen Percentage (valence electron model)

The hydrogen in the sample has been obtained from the valence electron model and it is a function of dispersion energy (E_d) and number of free valence electron (n_v). To obtain the error in the hydrogen content, it is a must to obtain the error for E_d and n_v . E_d is obtained from the slope (m) and intercept (c) of the linear portion of the plot of $(1 / n^2 - 1)$ versus $(h\nu)^2$.

$$E_d = \sqrt{\frac{c}{m}}$$

$$\left[\frac{\Delta c}{c} \right] = 6.21 \times 10^{-3}$$

$$\left[\frac{\Delta m}{m} \right] = 2.48 \times 10^{-3}$$

$$\left[\frac{\Delta E_d}{E_d} \right]^2 = \left[\frac{\Delta c}{c} \right]^2 + \left[\frac{\Delta m}{m} \right]^2 = 4.47 \times 10^{-5}$$

$$\left[\frac{\Delta E_d}{E_d} \right] = 6.69 \times 10^{-3}$$

$$n_v = 0.0143 \frac{E_d^2}{\epsilon(0) - 1} \times 10^{23}$$

$$\epsilon_0 = n^2 (1100)$$

where ;

$$\left[\frac{\Delta n_v}{n_v} \right]^2 = 2 \left[\frac{\Delta E_d}{E_d} \right]^2 + 4 \left[\frac{\Delta n}{n} \right]^2$$

$$\left[\frac{\Delta n_v}{n_v} \right]^2 = 0.01$$

$$\left[\frac{\Delta n_v}{n_v} \right] = 0.1$$

Hydrogen percentage in the sample,

$$C_H = \frac{1}{3} \frac{n_v}{n_s} \left(4 - \sqrt{\frac{E_d}{2.8}} \right) \times 100$$

$$\left[\frac{\Delta C_H}{C_H} \right]^2 = \left[\frac{\Delta n_v}{n_v} \right]^2 + \frac{1}{2} \left[\frac{\Delta E_d}{E_d} \right]^2$$

$$\left[\frac{\Delta C_H}{C_H} \right]^2 = 0.01$$

$$\left[\frac{\Delta C_H}{C_H} \right] = 0.1$$

B. 4 Optical Energy Gap (E_g)

From the intercept and slope of the plot of $(\alpha h\nu)^{1/2}$ versus $(h\nu)$, the optical energy gap has been deduced as :

$$E_g = \frac{c}{m}$$

where c is the intercept on y-axis and m is the gradient of the linear portion of the above plot,

$$\left[\frac{\Delta E_g}{E_g} \right]^2 = \left[\frac{\Delta c}{c} \right]^2 + \left[\frac{\Delta m}{m} \right]^2$$

$$\left[\frac{\Delta E_g}{E_g} \right]^2 = (2.329 \times 10^{-4}) + (1.463 \times 10^{-5})$$

$$\left[\frac{\Delta E_g}{E_g} \right] = 0.01$$

B. 5 Width Of The Band Tail (E_g)

The error in the width of the band tail has to be obtained by using the following equation;

$$\alpha = \exp \left[\frac{E}{E_g} \right]$$

$$\ln(\alpha) = \left[\frac{E}{E_g} \right]$$

From the equation E_g has to be obtained from the gradient in the linear portion of graph $\ln(\alpha)$ versus $(h\nu)$ and m is the slope of the graph in the linear portion,

$$E_g = \frac{1}{m}$$

$$E_g = m^{-1}$$

$$\left[\frac{\Delta E_g}{E_g} \right]^2 = \left[\frac{\Delta m}{m} \right]^2$$

$$\left[\frac{\Delta E_g}{E_g} \right] = \left[\frac{\Delta m}{m} \right]$$

$$\left[\frac{\Delta E_g}{E_g} \right] = 0.02$$

B. 6 D. C. Conductivity

$$\sigma = \frac{I}{V} \frac{d}{A} = (\text{slope}) \frac{d}{wt}$$

$$\left[\frac{\Delta \sigma}{\sigma} \right]^2 = \left[\frac{\Delta \text{slope}}{\text{slope}} \right]^2 + \left[\frac{\Delta d}{d} \right]^2 + \left[\frac{\Delta w}{w} \right]^2 + \left[\frac{\Delta t}{t} \right]^2$$

$$\left[\frac{\Delta\sigma}{\sigma} \right]^2 = 2.46 \times 10^{-5} + 0.0012 + 2.3 \times 10^{-6} + 6.85 \times 10^{-5}$$

$$\left[\frac{\Delta\sigma}{\sigma} \right]^2 = 0.001295$$

$$\left[\frac{\Delta\sigma}{\sigma} \right] = 0.04$$

B. 7 Activation Energy ($E_c - E_f$)

$$E_c - E_f = k \times S_1$$

where S_1 is the gradient of the first slope,

$$\left[\frac{\Delta(E_c - E_f)}{(E_c - E_f)} \right] = \left[\frac{\Delta S_1}{S_1} \right] = 0.06$$

B. 8 Density Of States At Fermi Level

$$\sigma(\omega) = \frac{\pi}{3} e^2 k [N(E_f)]^2 \alpha^{-5} \omega \left[\ln \left(\frac{V_{ph}}{\omega} \right) \right]^5 T$$

$$\sigma(\omega) = A [N(E_f)]^2 T$$

where A is the constant value,

$$[N(E_f)]^2 = \frac{\sigma(\omega)}{AT}$$

$$[N(E_f)] = \left[\frac{\sigma(\omega)}{AT} \right]^{\frac{1}{2}} = \left[\frac{m}{A} \right]^{\frac{1}{2}}$$

where m is the gradient of the graph $\sigma(\omega)$ versus temperature (T),

$$\left[\frac{\Delta N(E_f)}{N(E_f)} \right]^2 = \frac{1}{2} \left[\frac{\Delta m}{m} \right]^2 = 3.18 \times 10^{-3}$$

$$\left[\frac{\Delta N(E_f)}{N(E_f)} \right] = 0.06$$

B. 9 Hydrogen Percentage from FTIR

To obtain the error in the hydrogen percentage from FTIR calculation, it is a must to obtain the error for integrated intensity (I) and area under the curve (S).

$$I = \left[\frac{S}{w_0} \right]$$

where w_0 is the peak of the curve.

$$\left[\frac{\Delta I}{I} \right] = \left[\frac{\Delta S}{S} \right]$$

$$S = \left[\frac{22xA}{7xBB} \right]^{\frac{1}{2}}$$

where A is the intercept of the graph (α versus wavenumber) at y-axis and BB is the gradient of the graph in the linear region.

$$\left[\frac{\Delta S}{S} \right]^2 = \frac{1}{2} \left[\frac{\Delta A}{A} \right]^2 + \frac{1}{2} \left[\frac{\Delta BB}{BB} \right]^2$$

$$\left[\frac{\Delta S}{S} \right]^2 = 9.52 \times 10^{-9} + 4.84 \times 10^{-3}$$

$$\left[\frac{\Delta S}{S} \right] = 0.07$$

$$\left[\frac{\Delta I}{I} \right] = \left[\frac{\Delta S}{S} \right] = 0.07$$

$$\text{Hydrogen Content (C}_H\text{)} = 1.6 \times 10^{19} \times I$$

$$\left[\frac{\Delta C_H}{C_H} \right] = \left[\frac{\Delta I}{I} \right] = 0.07$$

B. 10 Oscillator Strength (Γ)

$$\Gamma = \left[37.6 \frac{I_{HS}}{I_{HW}} \right]$$

$$\left[\frac{\Delta \Gamma}{\Gamma} \right]^2 = \left[\frac{\Delta I_{HS}}{I_{HS}} \right]^2 + \left[\frac{\Delta I_{HW}}{I_{HW}} \right]^2$$

$$\left[\frac{\Delta \Gamma}{\Gamma} \right]^2 = 9.8 \times 10^{-3}$$

$$\left[\frac{\Delta \Gamma}{\Gamma} \right] = 0.09$$

B. 11 Parameter R

$$R = \frac{I_{2100}}{(I_{2000} + I_{2100})}$$

$$\left[\frac{\Delta R}{R} \right]^2 = \left[\frac{\Delta I_{2100}}{I_{2100}} \right]^2 + \left[\frac{\Delta I}{I} \right]^2$$

where,

$$\Delta I = \Delta I_{2000} + \Delta I_{2100}$$

$$I = I_{2000} + I_{2100}$$

$$\left[\frac{\Delta R}{R} \right] = 0.09$$

B. 12 Deposition Rate

$$\text{Deposition Rate} = \left[\frac{\text{Thickness}(d)}{\text{DepositionTime}(t)} \right]$$

$$\left[\frac{\Delta \text{Dep. Rate}}{\text{Dep. Rate}} \right]^2 = \left(\frac{\Delta d}{d} \right)^2 + \left(\frac{\Delta t}{t} \right)^2$$

$$\left[\frac{\Delta \text{Dep. Rate}}{\text{Dep. Rate}} \right]^2 = 8.27 \times 10^{-3} + 3.443 \times 10^{-10}$$

$$\left[\frac{\Delta \text{Dep. Rate}}{\text{Dep. Rate}} \right] = 0.09$$

Appendix C

Appendix C

Strong lines: 4.04/1 4.04/1 4.04/1 0.00/1 0.00/1 0.00/1 0.00/1 0.00/1

97 JCPDS-ICDD Copyright (c) 1995 PDF-2 Sets 1-45 database Quality: i

		d A	Int.	h	k	l
0						
2						
Titan Oxide						
		3.86	58	1	1	0
		3.71	22	0	2	0
		3.93	17	2	0	0
		5.42	9	-2	2	0
		4.571	9	1	1	1
d: CuK α	Lambda: 1.5418	Filter: Mono.	d-sp: Diff.			
toff:	Int: Diffractometer	I/Icor:				
f: Highcock, R., Smith, G., Wood, D., Acta Crystallogr., Sec. C, 4: 1391 (1985)						
		4.364	100	0	2	1
		3.676	66	2	2	1
		3.616	43	3	3	0
		3.464	31	4	0	0
		3.341	7	3	1	1
s: Orthorhombic	S.G.: Cmc21 (36)					
13.836(3)	b: 17.415(4)	c: 5.042(1)	A: 0.7945	C: 0.2895		
f: Ibid.			Z: 24	ap:		
	1.971	Dw:	SS/FOM: F28=9(.019,158)			
	nxB:	ay:	Sign:	2V:		
own from a gel. SiO ₂ :Al ₂ O ₃ = 60:1. PSC: aC72. Nwt: 60.08. Volume[CD]: 14.89.						
		2.365	4	2	6	1
		2.283	<1	2	2	2
		2.237	<1	5	3	1
		2.066	2	5	3	2
		2.035	2	4	6	1
		1.871	5	7	3	0
		1.784	2	3	9	0

d A	Int.	h	k	l	d A	Int.	h	k	l	d A	Int.	h	k	l
6025	4	1	3	3										
4546	2	0	6	3										
3829	2	7	9	0										

Strong lines: 4.36/1 3.68/7 10.9/6 3.62/4 3.46/3 3.30/3 8.71/2 6.93/2

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Quality: *

		d Å	Int.	h	k	l
Si:						
Silicon		3.1355	100	1	1	0
		1.9201	55	2	2	0
		1.6375	30	3	1	1
Silicon, syn		1.3577	6	4	0	0
		1.2459	11	3	3	1
Rad: CuKα	Lambda: 1.540598	Filter: Mono.	d-sp: Diff.			
Cutoff:	Int: Diffractometer	I/I ₀ : 4.70				
Ref: Natl. Bur. Stand. (U.S.) Monogr. 25, 13 35 (1976)						
		1.1086	12	4	2	2
		1.0452	6	5	1	1
		0.9600	3	4	4	0
		0.9180	7	5	3	1
		0.8587	8	6	2	0
Sys: Cubic	S.G.: Fd3m (227)					
a: 0.35889(4)	b:	c:	A:	C:		
A:	B:	C:	Z: 8	mp:		
Ref: Ibid.						
D ₀₄ : 2.33	D ₀₂ :	SS/FOM: F11=409(1.002,13)				
ω:	ωω2:	εy:	Sign:	2V:		
φ:						
Color: Gray						
Pattern taken at 25(1) °C. This sample is NBS Standard Reference Material No. 640. CAS no.: 7440-21-3. Reflections calculated from precision measurement of a ₀ . a ₀ uncorrected for refraction. C type. Diamond group. W used as internal standard. PSC: cFB. To replace 5-565 and 26-1481. Mwt: 28.09. Volume(CD): 160.18.						

Strong lines: 3.14/1 1.92/6 1.64/3 1.11/1 1.25/1 0.86/1 0.92/1 1.36/1