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APPENDICES

APPENDIX A

CALCULATION OF THE CRYSTALLITE SIZE

Calculation of the crystallite size by Debye-Scherrer equation

The crystallite size was calculated from the half-height width of the diffraction peak of XRD pattern using the Debye-Scherrer equation.

From Scherrer equation:

$$D = \frac{K\lambda}{\beta \cos \theta} \qquad \text{(B.1)}$$

where D = Crystallite size, Å

K = Crystallite-shape factor = 0.9

λ = X-ray wavelength, 1.5418 Å for CuKα

θ = Observed peak angle, degree

β = X-ray diffraction broadening, radian

The X-ray diffraction broadening (β) is the pure width of a powder diffraction free of all broadening due to the experimental equipment. Standard α-alumina is used to observe the instrumental broadening since its crystallite size is larger than 2000 Å. The X-ray diffraction broadening (β) can be obtained by using Warren's formula.

From Warren's formula:

$$\beta^2 = B_M^2 - B_S^2 \qquad \text{(B.2)}$$

$$\beta = \sqrt{B_M^2 - B_S^2}$$

Where B_M = The measured peak width in radians at half peak height.

B_S = The corresponding width of a standard material.

Example: Calculation of the crystallite size of titania

The half-height width of 101 diffraction peak = 0.93125°

= 0.01625 radian

The corresponding half-height width of peak of α-alumina = 0.004 radian

The pure width = $\sqrt{B_M^2 - B_S^2}$

= $\sqrt{0.01625^2 - 0.004^2}$

= 0.01577 radian

β = 0.01577radian

2θ = 25.56°

θ = 12.78°

λ = 1.5418 Å

The crystallite size = $\frac{0.9x\,1.5418}{0.01577\ \cos 12.78}$ = 90.15Å

= 9 nm

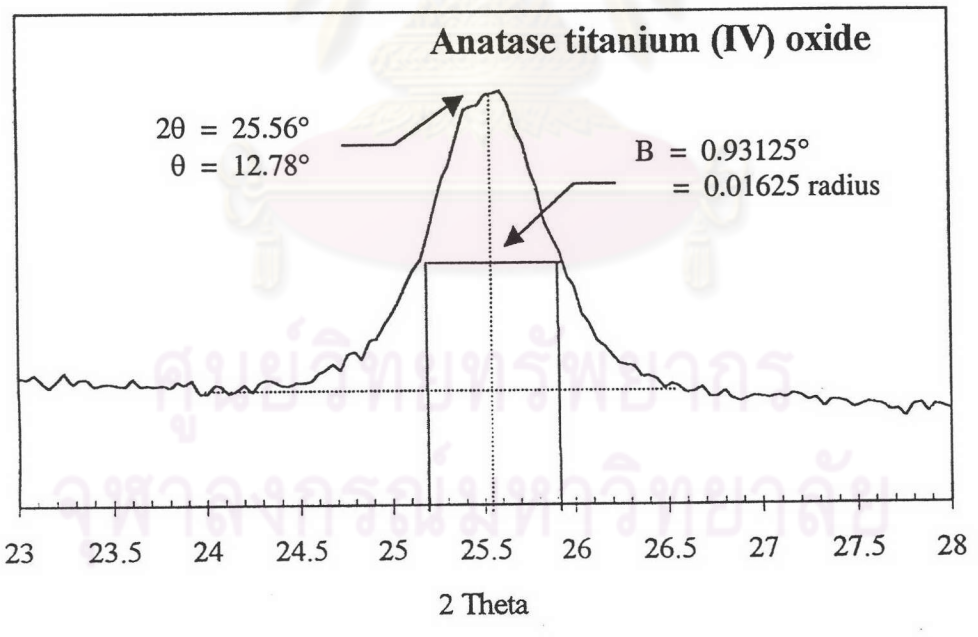

Figure A.1 The 101 diffraction peak of titania for calculation of the crystallite size

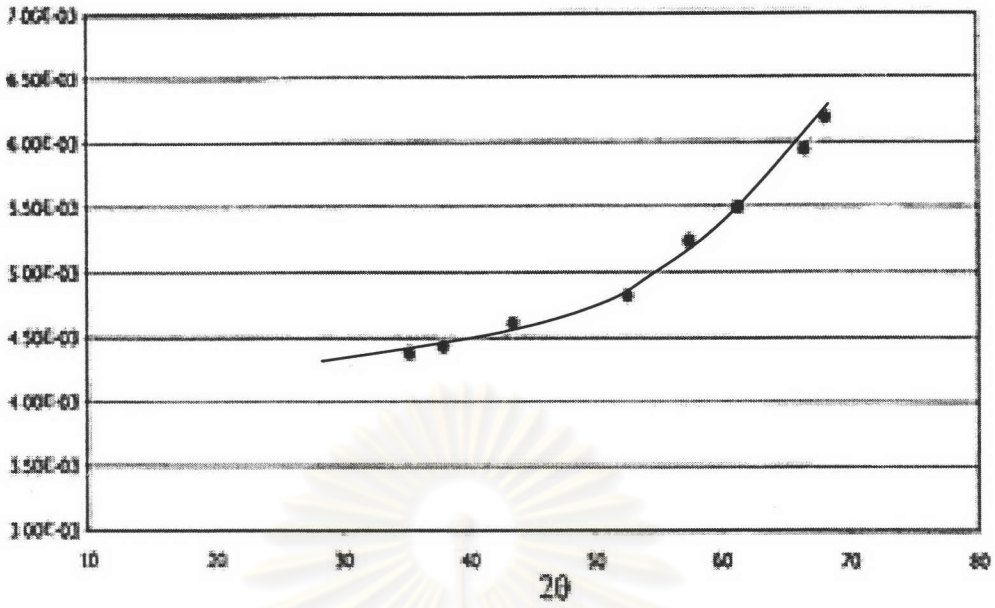

Figure A.2 The plot indicating the value of line broadening due to the equipment. The data were obtained by using α-alumina as standard

APPENDIX B

THE OPERATING CONDITIONS OF GAS CHROMATOGRAPHY

The composition of hydrocarbons in the product stream was analyzed by a Shimadzu GC14B gas chromatograph equipped with a flame ionization detector. The operating conditions for each instrument are shown in the Table B.1.

Table B.1 The operating condition for gas chromatograph.

Gas Chromagraph	SHIMADZU GC-14B
Detector	FID
Column	VZ10
Carrier gas	H_2 (99.999%)
Carrier gas flow (ml/min)	30 cc/min
Column temperature	
- initial (^oC)	70
- final (^oC)	70
Injector temperature (^oC)	100
Detector temperature (^oC)	150
Current (mA)	-
Analysed gas	Hydrocarbon C_1-C_4

The calibration curves for calculation of composition of reactant in photocatalytic reaction. The reactant is ethylene.

The VZ10 column are used with a gas chromatography equipped with a flame ionization detector, Shimadzu modal 14B, to analyze the concentration of products including of ethylene.

Mole of reagent in y-axis and area reported by gas chromatography in x-axis are exhibited in the curves. The calibration curves of ethylene is illustrated in the following figure.

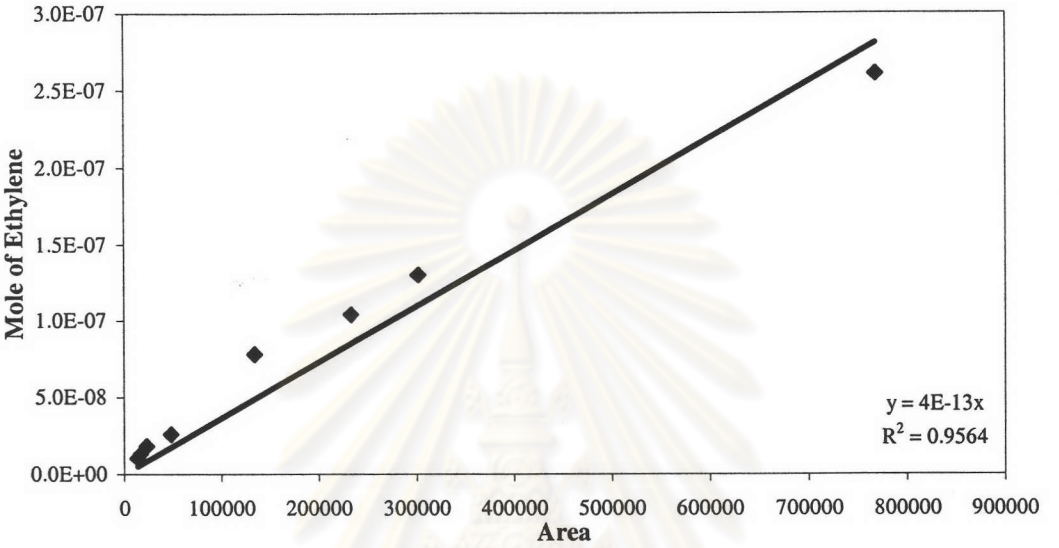

Figure B.1 The calibration curve of ethylene.

VITA

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