

Supplementary Materials: Photocatalytic Degradation of Acid Orange 7 by NiO-TiO₂/TiO₂ Bilayer Film Photo-Chargeable Catalysts

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Structural properties obtained from XRD data calculation

The structural properties of crystallite sizes (D), strain (ϵ), and dislocation density (δ) of BLF photocatalysts were calculated using the XRD data with the method from Igenepo John, et al. [1], Khot, et al. [2], and Goktas, et al. [3]. Debye-Scherrer equation (Eq. (1)) was used to estimate the size of crystal

$$D = \frac{K\lambda}{\beta \cos \theta} \quad (1)$$

where D is crystallite size in nm, K is the Scherrer constant, 0.94. λ represents the X-ray wavelength, which is from CuK α at 0.154 nm. β is a full width half maximum (FWHM) of a peak at Bragg's angle (θ).

Microstrain and dislocation energy were calculated using equations (2) and (3), respectively.

Citation: Wongburapachart, C.; Pornaroontham, P.; Kim, K.; Rangsunvigit, P. Photocatalytic Degradation of Acid Orange 7 by NiO-TiO₂/TiO₂ Bilayer Film Photo-Chargeable Catalysts. *Coatings* **2023**, *13*, 141. <https://doi.org/10.3390/coatings13010141>

Academic Editors: Jumei Li and Alexandru Enesca

Received: 12 December 2022

Revised: 6 January 2023

Accepted: 9 January 2023

Published: 10 January 2023



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$$\varepsilon = \frac{\beta}{4 \tan \theta} \quad (2)$$

$$\delta = \frac{1}{D^2} \quad (3)$$

In addition, the lattice constants of TiO₂ and NiO phases were determined by using equation below:

$$\frac{1}{d_{hkl}^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} \quad (4)$$

where d_{hkl} is the interplanar distance, and h, k, l are the Miller indices. For anatase TiO₂, which is a tetragonal crystal, the lattice constants are $a = b \neq c$, while NiO, a face-centered cubic, has the lattice constants of $a = b = c$.

Table S1. Average crystallite size, microstrain, dislocation density, lattice constants, and volume cell of BLF photocatalysts.

Sample	TiO ₂ Anatase			Lattice constants			NiO phase			Lattice constants	
	D_{average}	ε	δ	$a=b$	c	Volume cell	D_{average}	ε	δ	$a=b=c$	Volume cell
	(nm)	(#/nm ²)	(Å)	(Å)	(Å)	(Å ³)	(nm)	(#/nm ²)	(Å)	(Å)	(Å ³)
39-300BLF	12.16	0.0103	0.0068	3.784	9.465	135.49	6.61	0.0141	0.0229	4.178	72.95
52-300BLF	13.43	0.0094	0.0055	3.779	9.543	136.29	6.12	0.0152	0.0267	4.178	72.94
62-300BLF	15.66	0.0088	0.0041	3.776	9.446	134.64	7.04	0.0132	0.0202	4.178	72.92
69-300BLF	16.20	0.0081	0.0038	3.784	9.348	133.83	6.44	0.0144	0.0241	4.173	72.67
52-250BLF	9.14	0.0136	0.0120	3.780	9.402	134.36	5.47	0.0170	0.0334	4.176	72.84
52-350BLF	8.54	0.0148	0.0137	3.780	9.585	136.92	5.90	0.0158	0.0287	4.174	72.71
52-400BLF	9.29	0.0134	0.0116	3.784	9.348	133.83	7.12	0.0132	0.0197	4.181	73.08

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