Supporting Information for

Relationships Between Cell Parameters of Dye-sensitized Solar Cells and Dye-adsorption Parameters

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Estimating average crystallite dimensions of anatase nanocrystals

Average crystallite dimensions of anatase nanocrystals can be estimated from the line broadening of XRD diffraction peaks using Sherrer formula (1) .

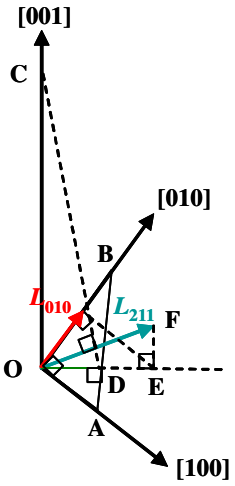
$L = k\lambda/\beta\cos\theta$ (1)

where L is the crystallite size, k is the Sherrer constant usually taken as 0.89, λ is the wavelength of X-ray radiation (0.15418 nm for Cu Kα), and β is the full width half maximum (FWHM) of diffraction peak measured at 2θ. The average crystallite dimensions of anatase in [100] and [001] directions can be estimated from diffraction data of (200) and (004) diffraction peaks, respectively.

Since all the anatase nanocrystals prepared here have thin plate-like morphology, they attach always on the microgrid surface by the basal planes, being vertical to the direction of TEM observation. The thickness of the crystals is difficult to be observed directly by TEM analysis. We tried to estimate the thickness from the FWHM data of diffraction peak (211) using formula (2).

$L_{(010)} = 0.4403L_{(211)}$ (2)

where $L_{(010)}$ is crystallite dimension in [010] direction, corresponding to the thickness of the plate-like crystals; $L_{(211)}$ is the crystallite dimension calculated from the XRD diffraction peak of (211) plane using the Sherrer formula (1); the parameter 0.4403 is obtained from the lattice parameters of anatase (Tetragonal, a=0.37852nm, c=0.95139nm), where lattice vectors have a relationship of $V_{[211]} = V_{[010]} + V_{[200]} + V_{[001]}$, and the length ratio ($L_{(010)}$ /$L_{(211)}$) of $V_{[010]}$ to $V_{[211]}$ can be calculated as 0.4403.



$\overline{OA} = a/2$

$\overline{OC} = c = 0.95139$ nm

$\overline{OB} = b = a = 0.37852$ nm

$2\overline{OD}\sqrt{a^2/4 + a^2} = a^2$

$\overline{OD} = a\sqrt{5}/5$

$\angle BOE = r = 63.435^o$

$(\cos r = \overline{OD}/\overline{OB} = \sqrt{5}/5)$

$\angle CDO = \angle OFE = B = 79.916^o$

$(\sin B = c/\sqrt{c^2 + \overline{OD}^2})$

$\overline{OE} = L_{211} \sin B$

$L_{010} = \overline{OE} \cos r = L_{211} \sin B \cos r = 0.4403 L_{211}$

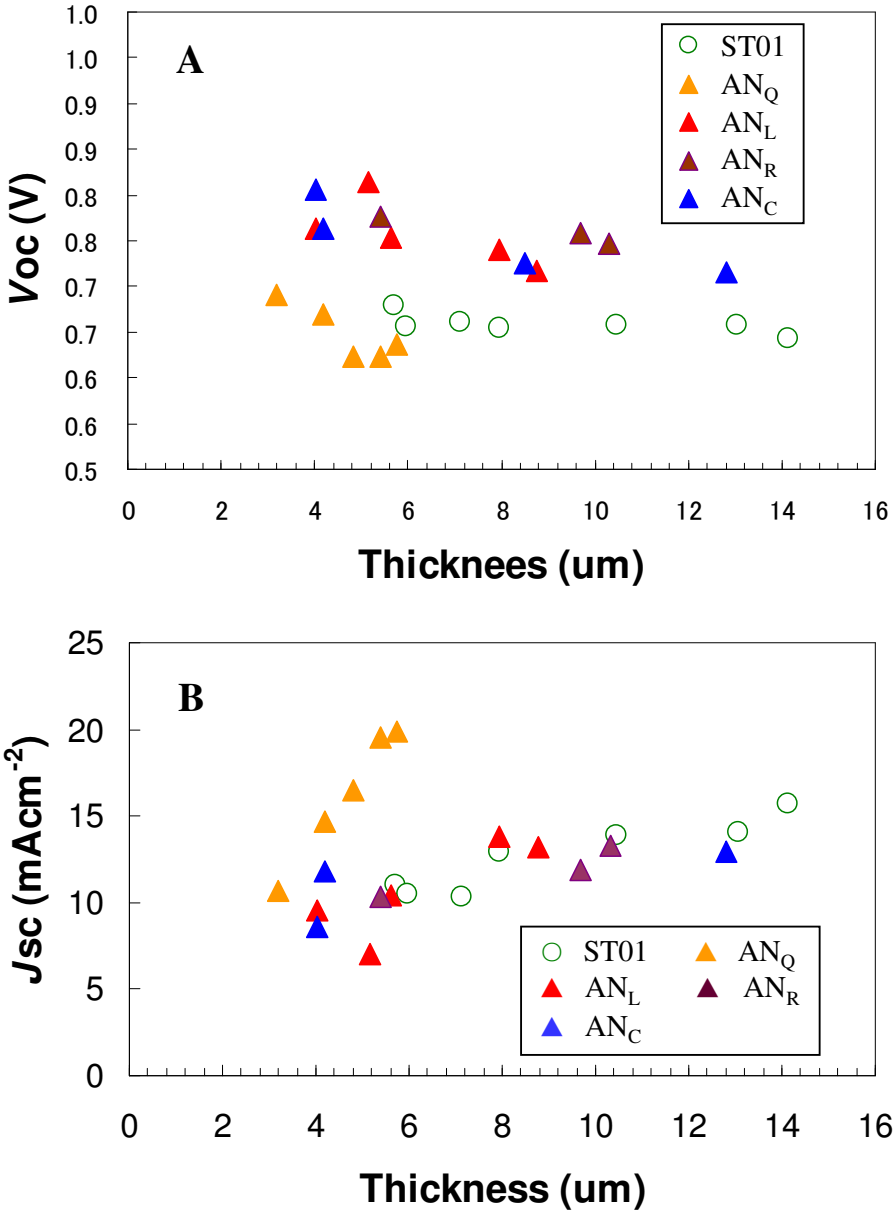


Figure S1. Dependences of the cell parameters on the TiO_2 film thickness for the DSCs prepared using TiO_2 nanocrystal samples. (**A**) Relationship between the open-circuit potential V_{oc} and the film thickness. (**B**) Relationship between the short-circuit current density J_{sc} and the film thickness. The V_{oc} slightly decreases about 3% with increase of the film thickness, but the decrease is small and can be ignored in the thickness region of 8 to 13μm for ST01 sample. The J_{sc} increases with increasing the film thickness up to 8 μm, and then keeps almost constant in the thickness region of 8 to 13μm. These results suggest that the relatively small variations of the V_{oc} and J_{sc} values can be obtained in the thickness region of 8 to 13μm.

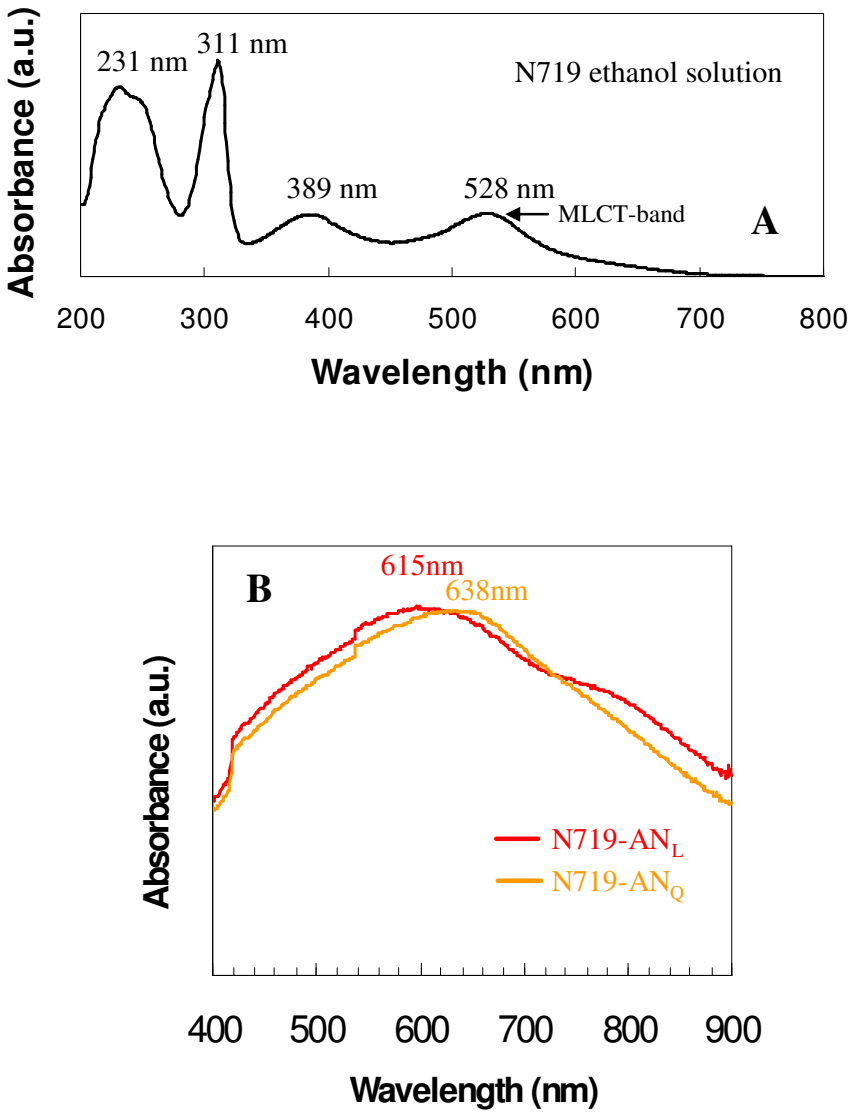


Figure S2. UV-Vis absorption spectra of (A) N719 in ethanol solution; (B) N719 adsorb-binding on the surface of AN_L and AN_Q samples.