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Supporting information for article:

Three-dimensional morphology of anatase nanocrystals obtained from supercritical flow synthesis with industrial grade TiOSO₄ precursor

Jinlong Yu, Frederik Søndergaard-Pedersen, Aref Mamakhe, Paolo Lamagni and Bo Brummerstedt Iversen

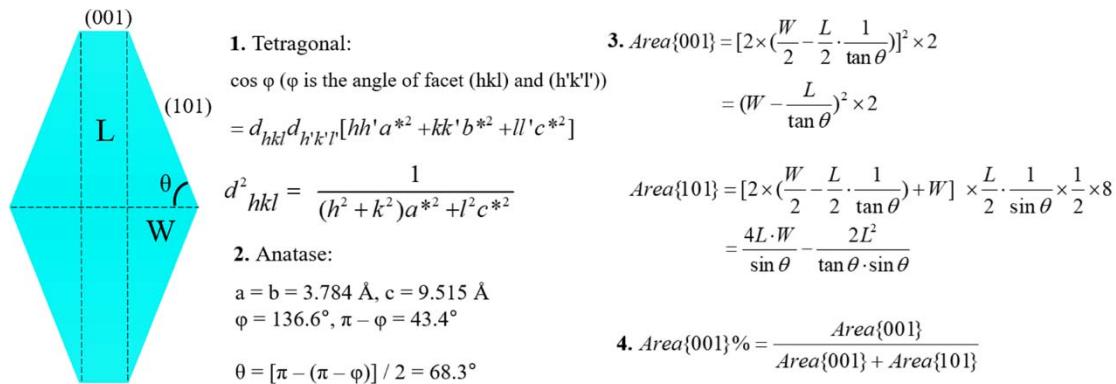
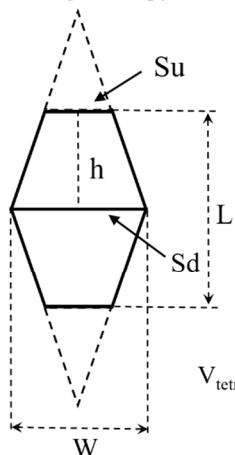


Figure S1. Schematic drawing of the truncated tetragonal bipyramidal model of a-TiO₂ nanocrystals utilized for calculating the percentage of exposed {001} facets.

Tetragonal bipyramidal

 S_u : area of the upper surface

$$S_u = \left[2 \times \left(\frac{W}{2} - \frac{L}{2} \times \frac{1}{\tan\theta} \right) \right]^2$$

 S_d : area of the down surface

$$S_d = W^2$$

$$h = \frac{L}{2}$$

$$V_{\text{tetragonal bipyramid}} = \frac{2h}{3} \times (S_d + S_u + \sqrt{S_d} \times \sqrt{S_u})$$

$$\text{Area}\{001\} = \left(W - \frac{L}{\tan\theta} \right)^2 \times 2$$

$$\text{Area}\{101\} = \frac{4 \times L \times W}{\sin\theta} - \frac{2 \times L^2}{\tan\theta \times \sin\theta}$$

$$S_{\text{total}} = \text{Area}\{001\} + \text{Area}\{101\}$$

For $\text{NH}_4\text{HCO}_3\text{-400 a-TiO}_2$:

$$L = 13.3 \text{ nm}, \quad W = 9.7 \text{ nm}$$

$$V = 699.2 \text{ nm}^3 \quad \rho = 3.78 \text{ g/cm}^3 \quad m = \rho \times V = 2.64 \times 10^{-18} \text{ g}$$

$$\text{Area}\{001\} = 39.1 \text{ nm}^2 \quad \text{Area}\{101\} = 406.4 \text{ nm}^2 \quad S_{\text{total}} = 445.5 \text{ nm}^2$$

$$\text{Specific surface area} = \frac{S_{\text{total}}}{V} = 168.5 \text{ m}^2/\text{g}$$

Figure S2. Specific surface area calculation process for $\text{NH}_4\text{HCO}_3\text{-400 a-TiO}_2$ sample.

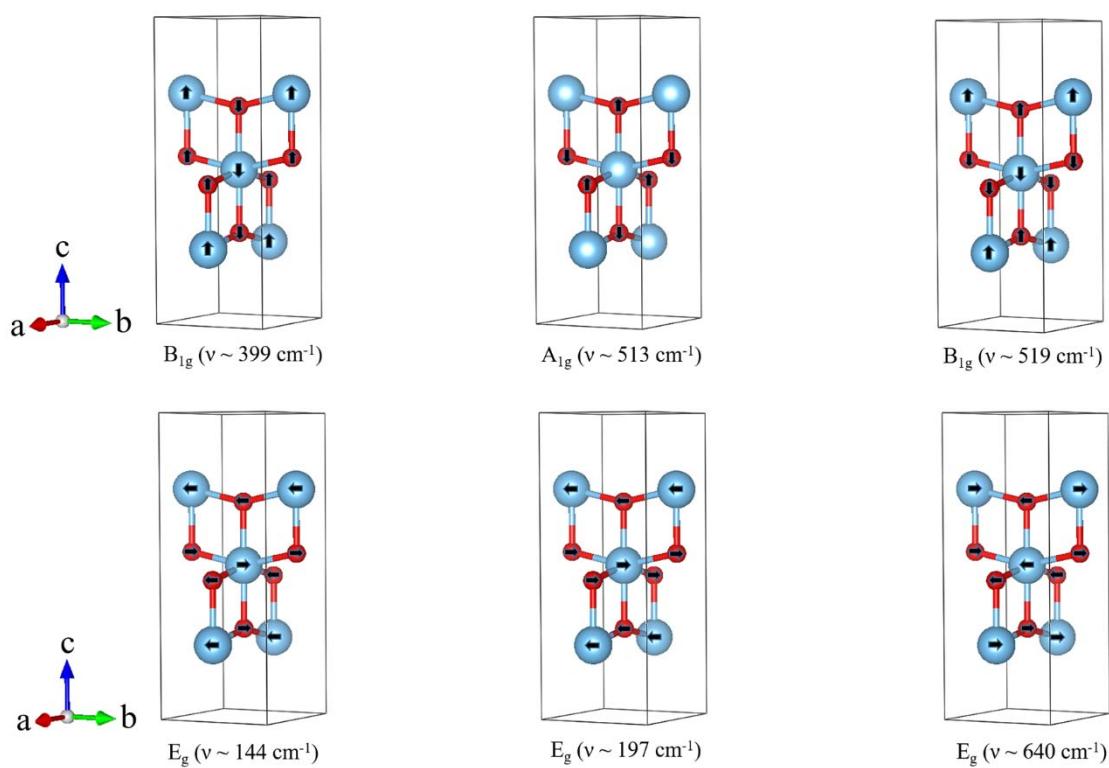


Figure S3. Schemes for different optical atomic vibrations in a-TiO₂ crystals according to Ohsaka et al (Ohsaka *et al.*, 1978). Red spheres represent the oxygen atoms while blue ones refer to titanium atoms.

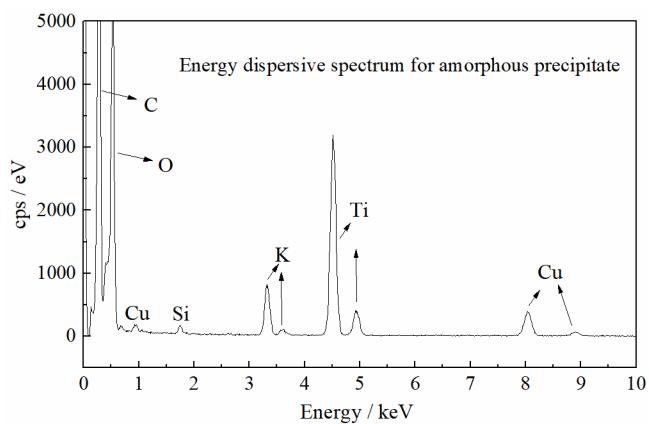


Figure S4. Energy dispersive X-ray spectrum of white compound obtained from neutralizing TiOSO₄ solution with 5 M KOH solution.

References

Ohsaka, T., Izumi, F. & Fujiki, Y. (1978). *J. of Raman Spectrosc.* **7**, 321- 324.