

# Supporting material

for

## **Continuous Flow Supercritical Water Synthesis and Crystallographic Characterization of Anisotropic Boehmite Nanoparticles**

Nina Lock,<sup>a</sup> Peter Hald,<sup>a</sup> Mogens Christensen,<sup>a</sup> Henrik Birkedal,<sup>b</sup> Bo Brummerstedt Iversen<sup>a\*</sup>

<sup>a</sup>Centre for Materials Crystallography, Department of Chemistry and iNANO, Aarhus University,  
Langelandsgade 140, DK-8000 Aarhus C, Denmark

<sup>b</sup>Department of Chemistry and iNANO, Aarhus University, Langelandsgade 140, DK-8000 Aarhus  
C, Denmark

\*Corresponding author: bo@chem.au.dk

### Refinements: spherical harmonics (refining $Y_{00}$ , $Y_{20}$ , $Y_{22+}$ , and $GauSiz$ )

The powder patterns refined using the spherical harmonic functions  $Y_{00}$ ,  $Y_{20}$ , and  $Y_{22+}$  and the Gaussian size component  $GauSiz$  are shown in Figure S1-S4. The grey circles are experimental data  $y(\text{obs})$ , the solid black line is the Rietveld model  $y(\text{calc})$ , and the grey line is  $y(\text{obs})-y(\text{calc})$ .

#### 300 bar/603 K:

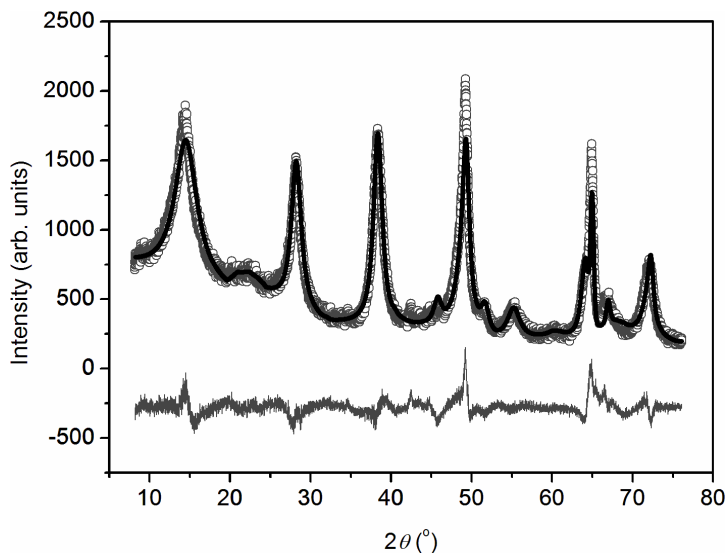


Figure S1. Powder diffraction data on the 300 bar/603 K sample refined using spherical harmonics.

#### 400 bar/603 K:

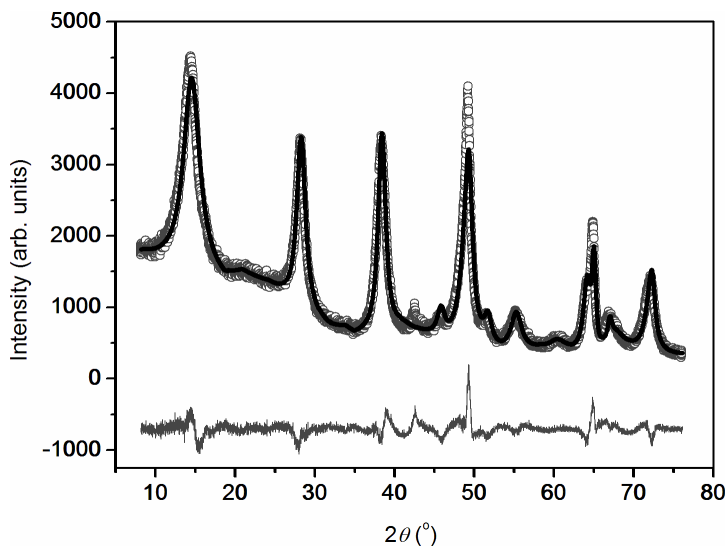


Figure S2. Powder diffraction data on the 400 bar/603 K sample refined using spherical harmonics.

**300 bar/693 K:**

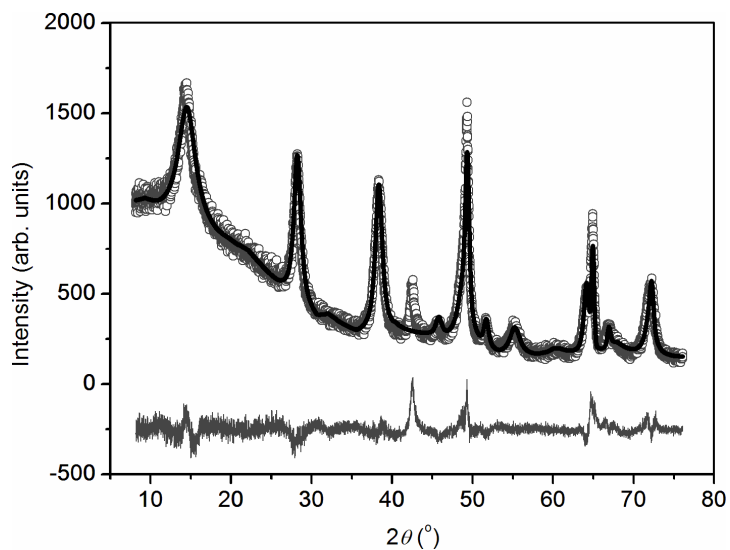


Figure S3. Powder diffraction data on the 300 bar/693 K sample refined using spherical harmonics.

**400 bar/693 K:**

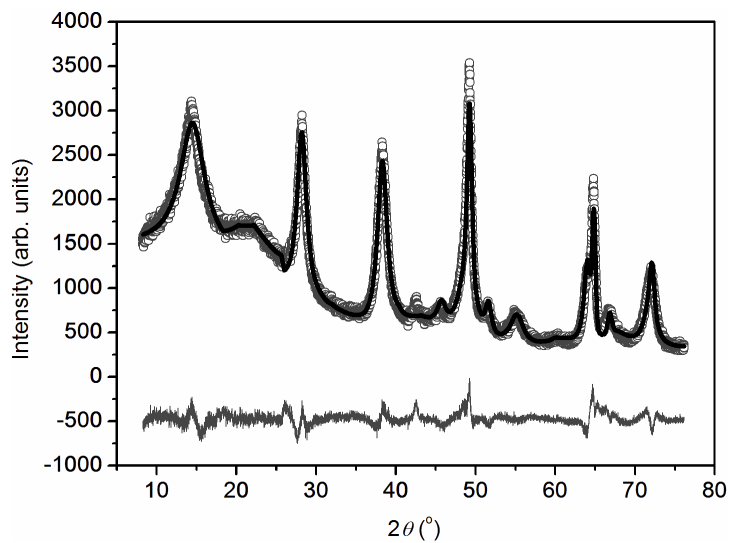


Figure S4. Powder diffraction data on the 400 bar/693 K sample refined using spherical harmonics.

The particle shape and particle sizes are shown in Figure S5.

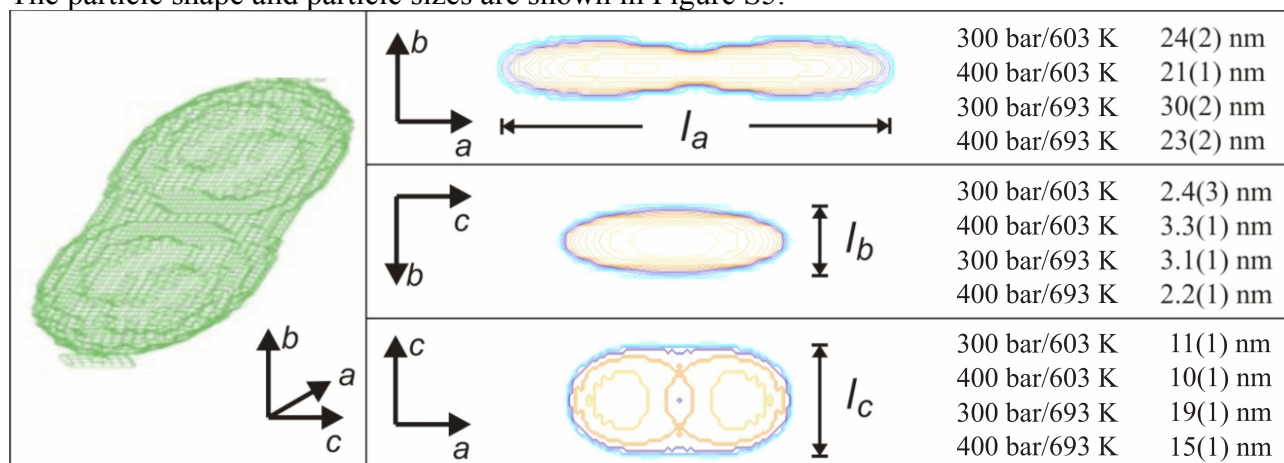


Figure S5. The crystallite shapes modeled by the spherical harmonic parameters visualized using the program GFourier contained in the FullProf Suite. The decrease in the particle size along the  $b$ -axis at the middle of the particle is likely to be caused by limitations in the collected data.

### Refinements: Quadratic Method (refining $h^2$ , $k^2$ , and $l^2$ )

The powder patterns refined using the quadratic function coefficients  $h^2$ ,  $k^2$ , and  $l^2$  are shown in Figure S6-S9. The grey circles are experimental data  $y(\text{obs})$ , the solid black line is the Rietveld model  $y(\text{calc})$ , and the grey line is  $y(\text{obs})-y(\text{calc})$ .

#### 300 bar/603 K:

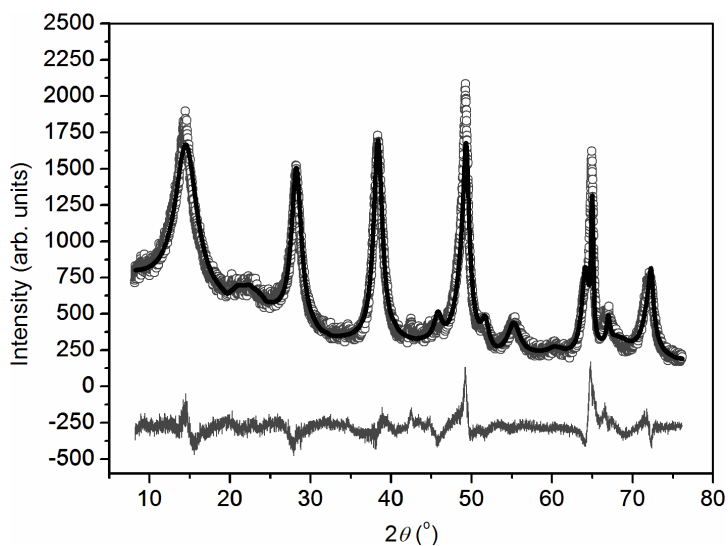


Figure S6. Powder diffraction data on the 300 bar/603 K sample refined using the quadratic method.

#### 400 bar/603 K:

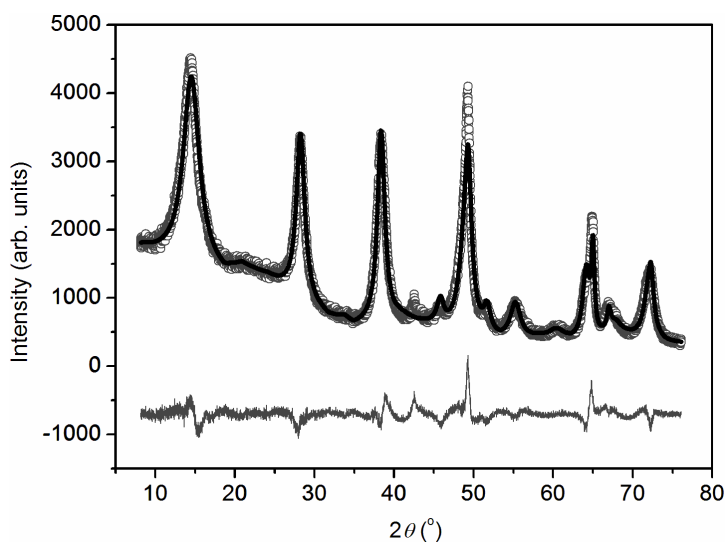


Figure S7. Powder diffraction data on the 400 bar/603 K sample refined using the quadratic method.

**300 bar/693 K:**

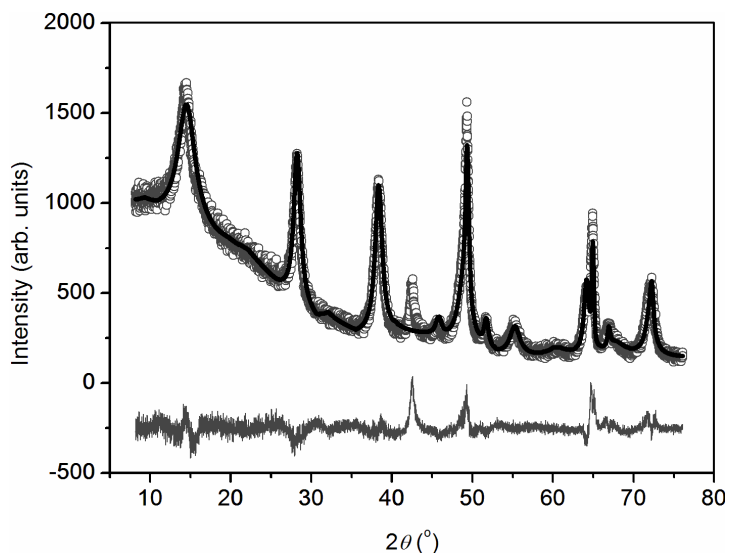


Figure S8. Powder diffraction data on the 300 bar/693 K sample refined using the quadratic method.

**400 bar/693 K:**

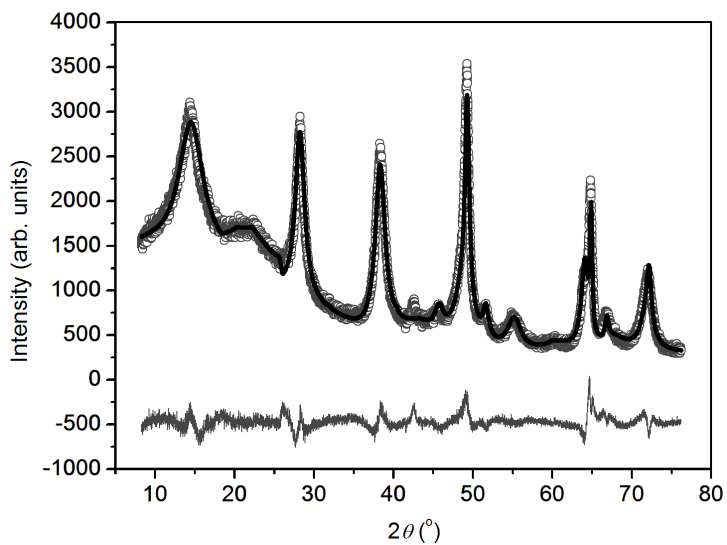


Figure S9. Powder diffraction data on the 400 bar/693 K sample refined using the quadratic method.

The particle shape and particle sizes are shown in Figure S10.

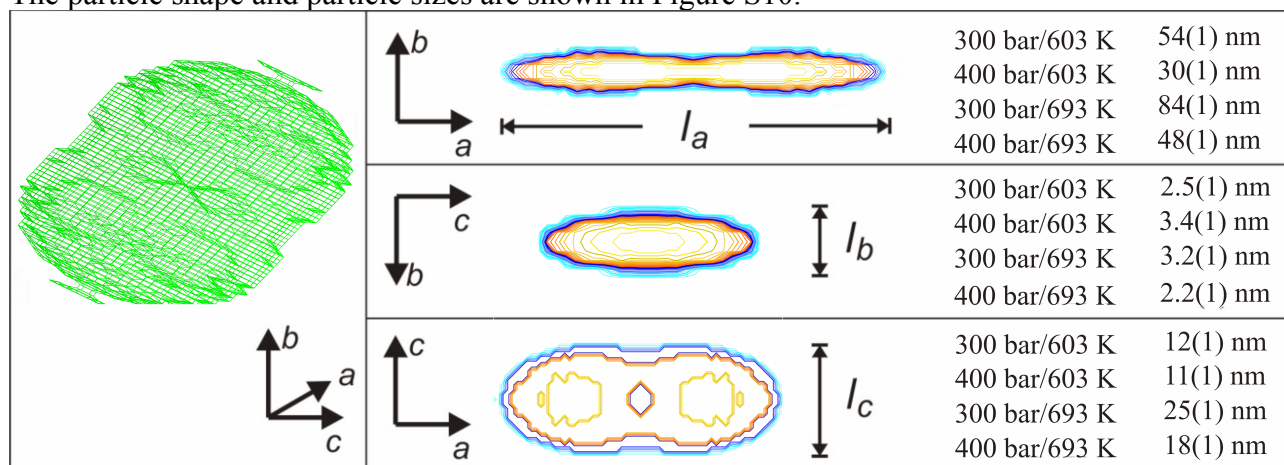


Figure S10. The crystallite shapes modeled by quadratic parameters visualized using the program GFourier contained in the FullProf Suite. The decrease in the particle size along the  $b$ -axis at the middle of the particle is likely to be caused by limitations in the collected data.