Electronic Supplementary Material (ESI) for Materials Advances.

Synthesis and characterization of nano-crystallite triple superphosphate from waste *Pila globosa* shells for sustainable industrial production

Md. Sahadat Hossain[a], Md. Aftab Ali Shaikh[a,b], Md. Farid Ahmed[a], Samina Ahmed[a,c*]*

[a]*Institute of Glass & Ceramic Research and Testing, Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka-1205, Bangladesh.*

[b]*Department of Chemistry, University of Dhaka, Dhaka-1000, Bangladesh.*

[c]*BCSIR Laboratories Dhaka, Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka-1205, Bangladesh.*

*Corresponding authors: shanta_samina@yahoo.com; aftabshaikh@du.ac.bd

Liner straight-line method of Scherrer's equation

The Liner straight-line model of the Scherrer's equation was also employed as the 2nd approach to calculate the crystallite size which is also based on the Scherrer's formula. The mathematical representation of the model can be written as equation 14 and the details are documented elsewhere.[1] The calculated crystallite size from this model was 1386 nm and the graphical illustration is shown in Figure 5. The too large calculated crystallite size made this mode invalid for the synthesized triple super phosphate.

$$Straight-line\ method: \cos(\theta) = \frac{K\lambda}{D_L} \times \frac{1}{\beta} \qquad (S\_1)$$

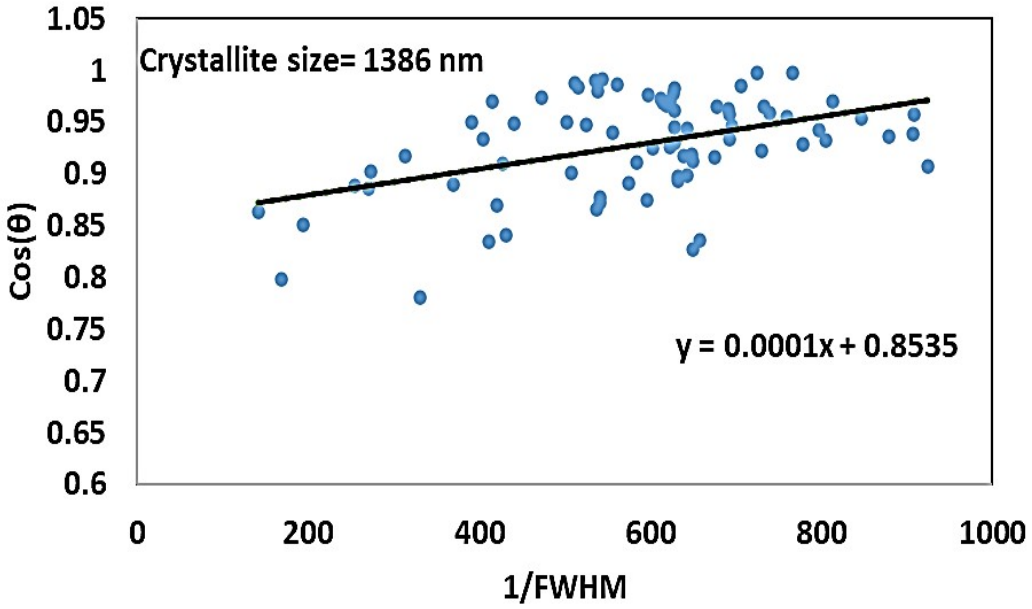

Figure S_1: Crystallite size of triple superphosphate using Liner straight-line method of Scherrer's equation

Three peaks model

$$\theta_{Average} = \frac{\theta_{peak-1} + \theta_{peak-2} + \theta_{peak-3}}{3} \qquad (S\_2)$$

$$\lambda_{Average} = \frac{\lambda_{K-\propto 1} + \lambda_{K-\propto 2}}{2} \qquad (S\_3)$$

$$FWHM_{Average} = \frac{FWHM_{peak-1} + FWHM_{peak-2} + FWHM_{peak-3}}{3} \qquad (S\_4)$$

$$Crystallite\ size, Daverage = \frac{K\lambda_{average}}{FWHM_{average}\, cos\theta_{average}} \qquad (S\_5)$$

Monshi–Scherrer model

$$Monshi\text{–}Scherrer\ model, \ln\beta = \ln\frac{1}{\cos\theta} + \ln\frac{K\lambda}{D_{M-S}} \qquad (S\_6)$$

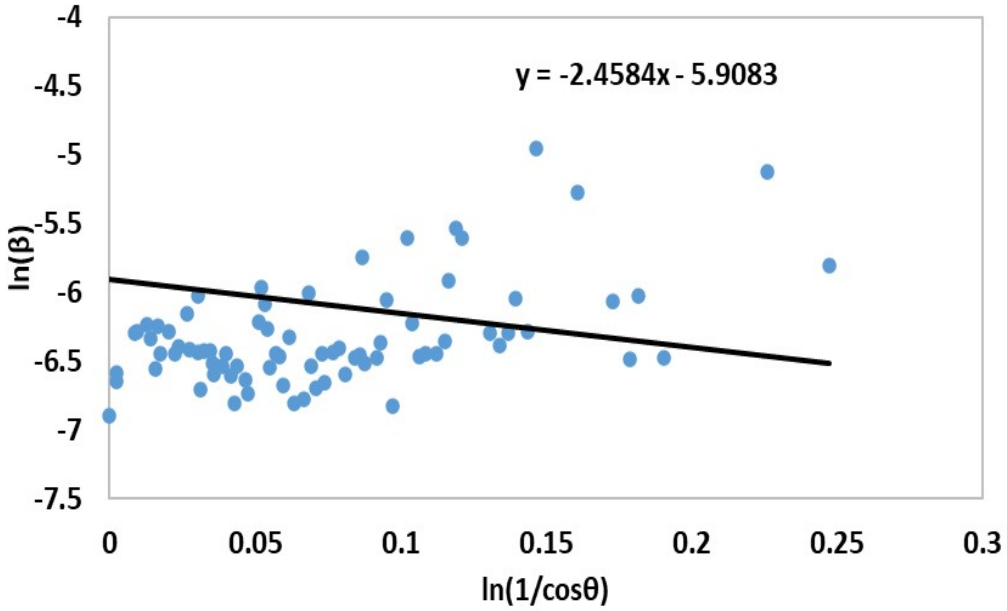

Figure S_2: Crystallite size of triple superphosphate using Monshi-Scherrer model

Williamson–Hall plot

The previously described models only consider the peak broadening from the crystal but this Williamson-Hall model include the instrumental broadening as well as broadening due to intrinsic strain. The crystallite size from the Scherrer's equation depends on the 1/cosθ but the Williamson–Hall plot is based on the tanθ which allows the separation of peak broadening due to the crystallite size as well as micro-strain.[2]

The Uniform Deformation Model (UDM) can be express as:

$$\beta_{total}\cos\theta = \frac{K_B\lambda}{D_{W-H}} + 4\,\varepsilon\,sin\theta \qquad (S\_7)$$

The Uniform Stress Deformation Model (USDM) can be presented as:

$$\beta_{total}\cos\theta = \frac{K_B\lambda}{D_{W-H}} + 4\,\frac{\sigma}{E_{hkl}}\,sin\theta \qquad (S\_8)$$

Uniform Deformation Energy Density Model (UDEDM) can be visualized as:

$$\beta_{total}\cos\theta = \frac{K_B\lambda}{D_{W-H}} + 4\,(\frac{2u}{E_{hkl}})^{1/2}\,sin\theta \qquad (S\_9)$$

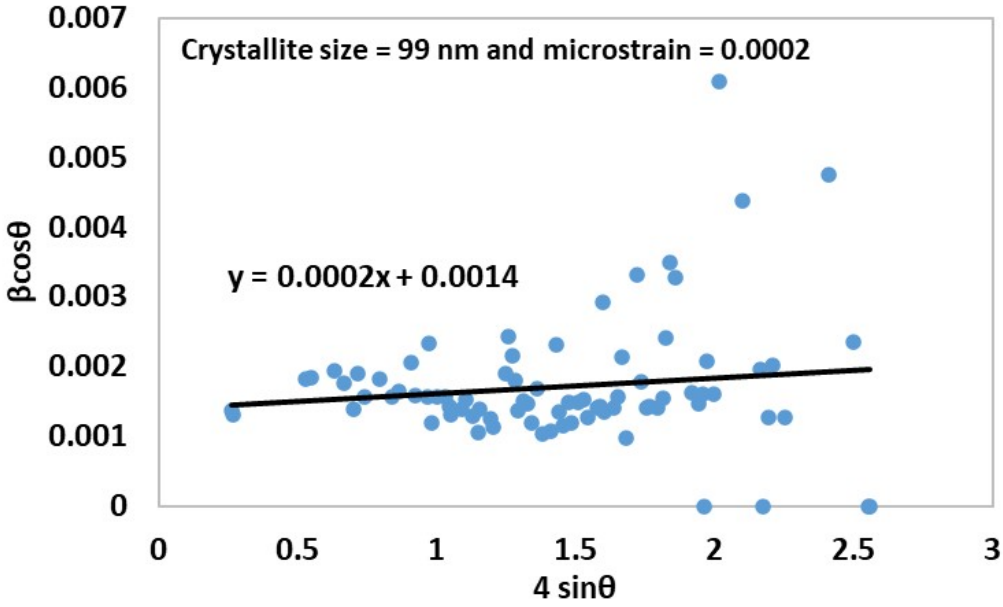

Figure S_3: Crystallite size calculation employing Uniform Deformation Model of Williamson-Hall plot

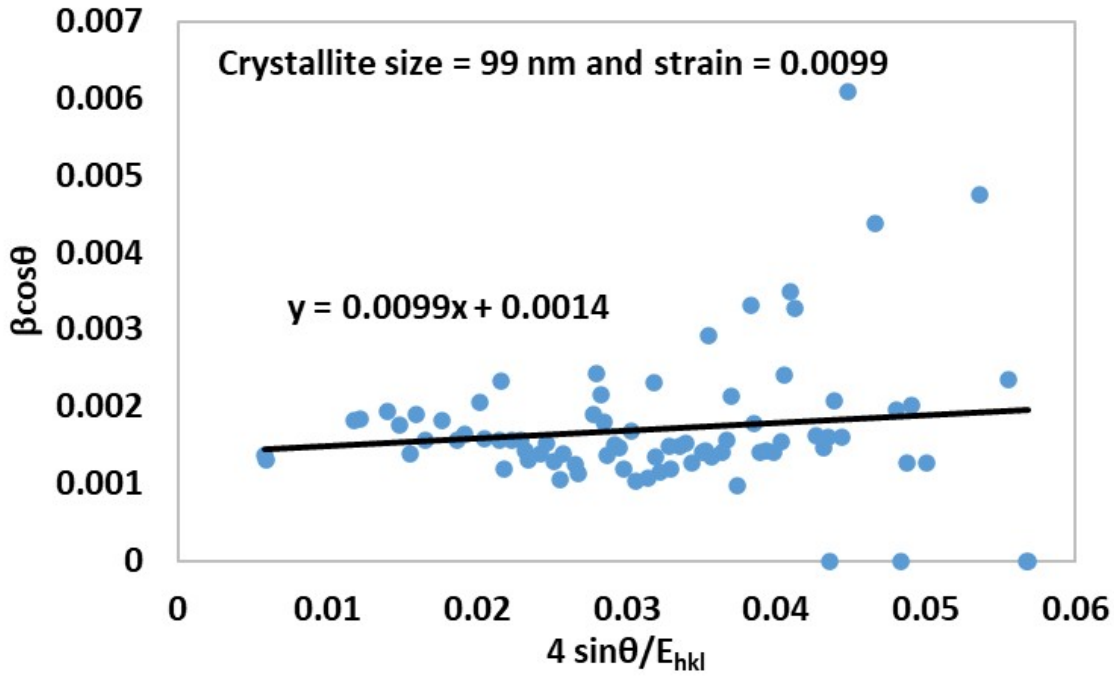

Figure S_4: Crystallite size calculation employing Uniform Stress Deformation Model of Williamson-Hall plot

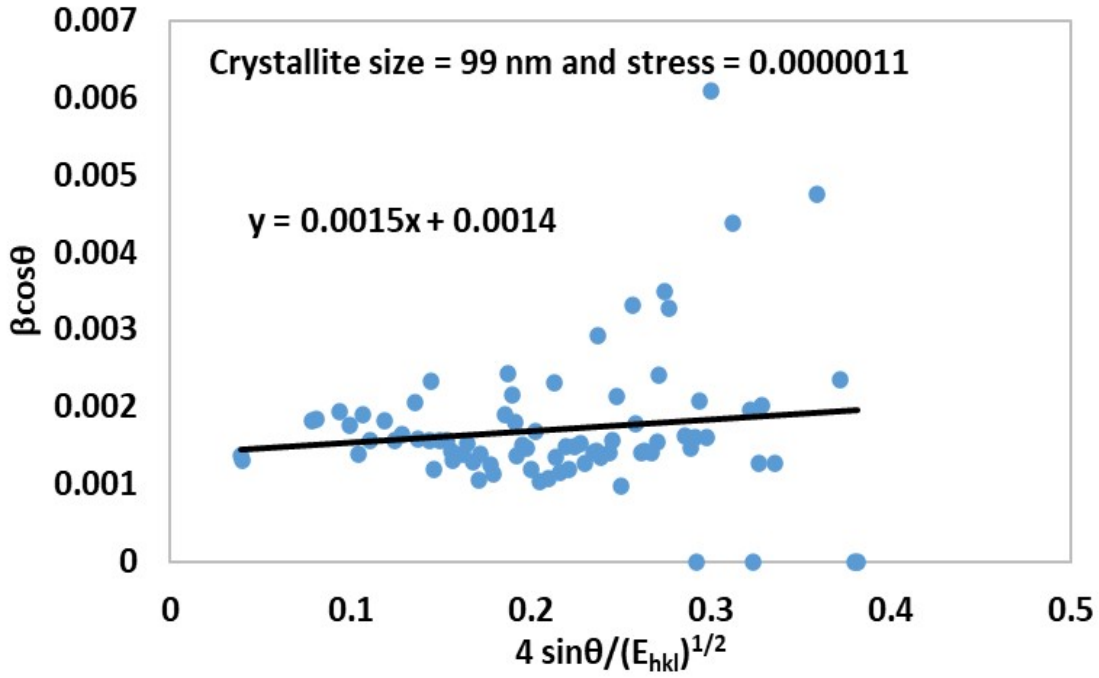

Figure S_5: Crystallite size calculation employing Uniform Energy density Deformation Model of Williamson-Hall plo

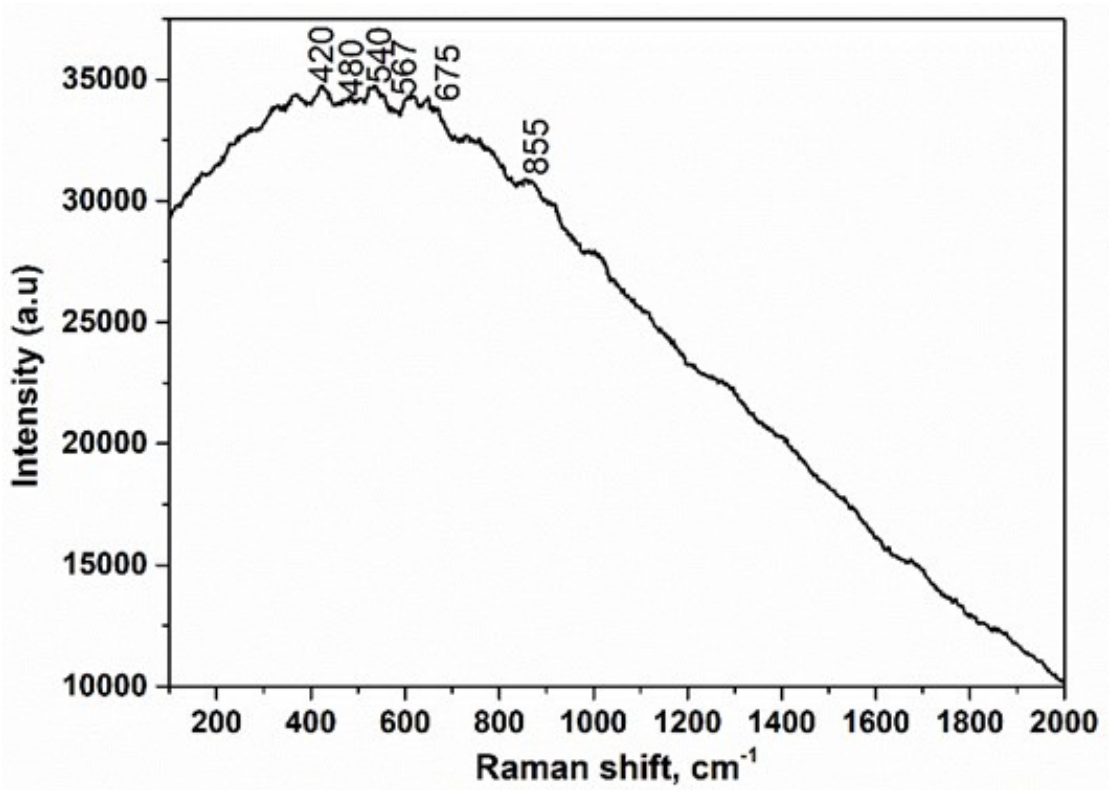

Figure S_6: Raman shift of synthesized triple super phosphate

References

1 M. S. Hossain, M. A. A. Shaikh, M. S. Rahaman and S. Ahmed, *Mol. Syst. Des. Eng.*, , DOI:10.1039/D2ME00061J.
2 D. Jamwal, G. Kaur, P. Raizada, P. Singh, D. Pathak and P. Thakur, *The Journal of Physical Chemistry C*, 2015, **119**, 5062–5073.