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Supporting information for article:

A numerical method for deriving shape functions of nanoparticles for pair distribution function refinements

Tedi-Marie Usher, Daniel Olds, Jue Liu and Katharine Page

An example implementing the numerical shape functions in TOPAS v6 is included as a TOPAS input file: **TOPAS_example.inp**. The Gaussian coefficients from Table 1. are included in the example script. The corresponding calculated PDF is included as **Au_10nm_tetra_corrected_pdf.xy**.

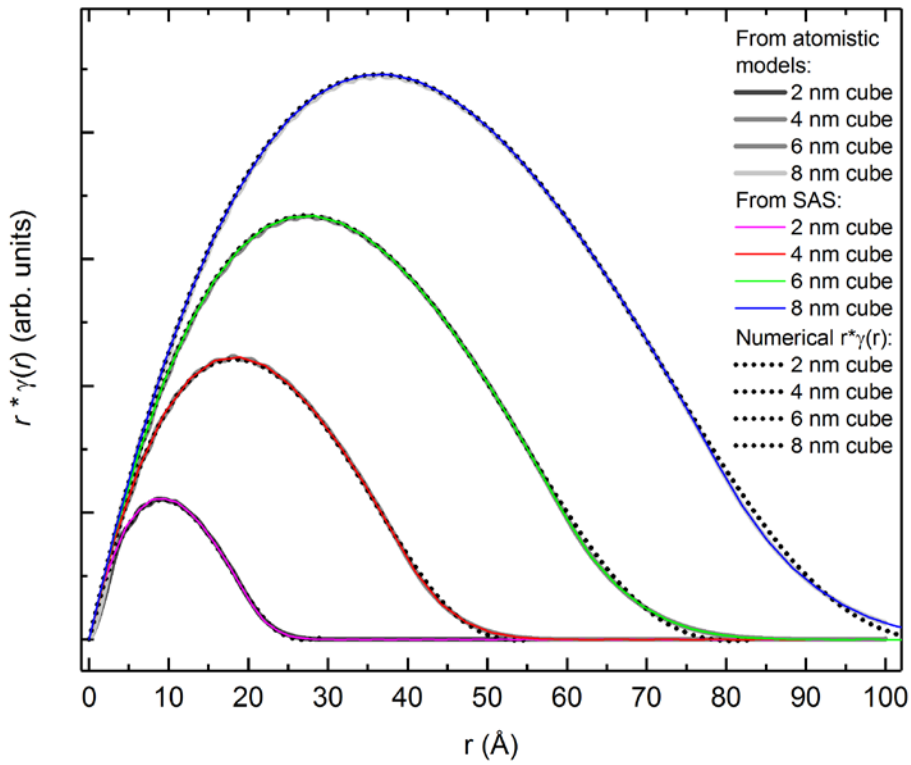

Figure S1 Comparison of shape functions for 2, 4, 6, and 8 nm cubes from various sources: atomistic models, SAS, and the numerical function presented in this work. Note that the numerical approximation is both fit and implemented in structural refinements as $\gamma(r)$, not $r \times \gamma(r)$, as shown in this figure.

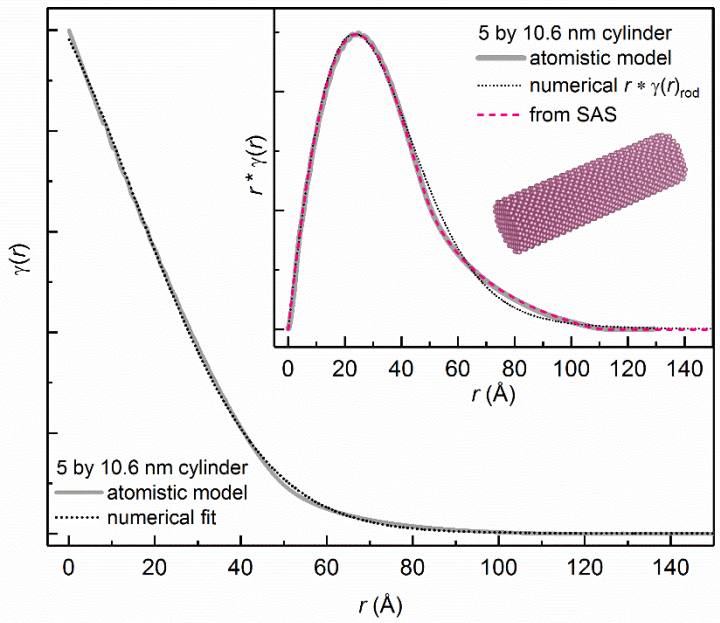

Figure S2 Comparison of shape functions for a cylinder with diameter of 5 nm and length of 10 nm from various sources: atomistic models, SAS, and the numerical function presented in this work. The inset shows the comparison in the form of $r \times \gamma(r)$, which amplifies the mismatch (due to the intrinsic limitation of using two Gaussian functions to fit a more complex shape function) between the numerical and other methods. However, in the $\gamma(r)$ form (how the numerical function is implemented in structural refinements), the mismatch is much smaller.

Shapes available in SasView:

- Cylinder
- Ellipsoid
- Lamellae
- Paracrystals (SCC, FCC, and BCC packing)
- Parallelepiped
- Sphere

Note that each category has multiple sub-shapes. E.g., the sphere model also contains fuzzy sphere, core-shell, linear pearls, etc., and the cylinder model contains a hollow cylinder, flexible cylinder, stacked disks, etc.

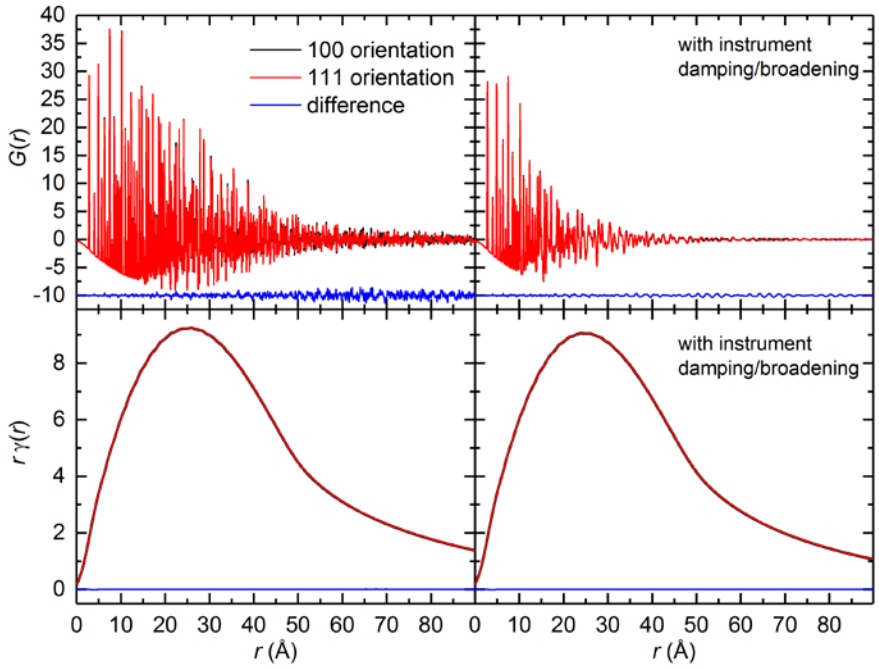

Figure S3 Atomistically calculated PDFs of Au nanorods (top panels) without damping and with realistic Q_{damp} and Q_{broad} instrument effects applied in DISCUS (0.008 Å^{-1} and 0.005 Å^{-1}, respectively) (Proffen & Neder, 1997). With or without instrument damping/broadening, the shape functions extracted from the PDFs of the rods with different crystallographic orientations have negligible differences (bottom panels).

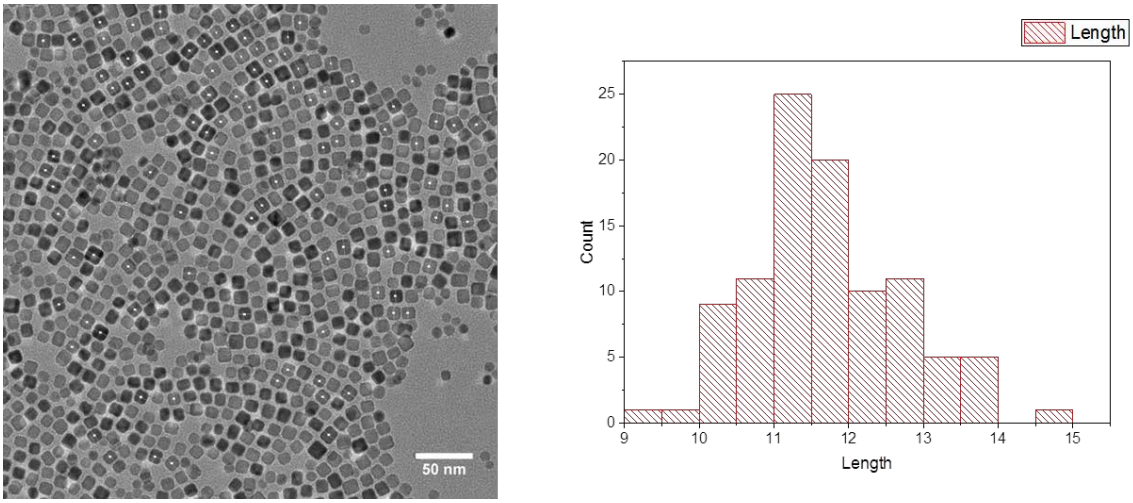

Figure S4 Transmission electron microscopy image of $BaTiO_3$ nanocubes (left) and a histogram of the edge length of 100 particles in the image (right). The particles used for the histogram analysis are marked with a white dot in the microscopy image, and have an average cube edge length of 11.8 nm, with a standard deviation of 1.1 nm.