

from the scattering by an icosahedral object. If so, the components of the quantities $B_l(q, q')$, derivable from the angular correlations, should have much smaller values for $l=1,2,3,4$, and 5 than for $l=0$ and $l=6$, for example. What is more, as we have shown in this paper, the coefficients $g_l(q)$ of the icosahedral harmonic expansion of the 3D diffraction volume of the particle may be derived from the $B_l(q, q')$ data and a positivity condition on the intensities of the 3D diffraction volume. This will be the case even if the individual diffraction patterns are a result of scattering from more than one particle, so there will be no need to discard the diffraction patterns from multiple particles.

Having obtained the coefficients of an icosahedral harmonic expansion, the 3D diffraction volume may be reconstructed as a sum over these icosahedral harmonics. By definition, the resulting diffraction volume will have icosahedral symmetry. If this is constructed at a grid that is oversampled by a factor of 2 in each dimension, we have shown that a “charge flipping” algorithm with no fixed support constraint is able to reconstruct a 3D image of the particle. We find that this procedure not only reconstructs an icosahedral shape for the particle, in simulations for the satellite tobacco necrosis virus (STNV) it even reveals the hollow nature of the protein coat.

Acknowledgments

We acknowledge helpful discussions with Profs. Abbas Ourmazd and John Spence, and financial support from DOE grant No. DE-SC0002141.