Characterization of Hierarchical Structures in Soft-Materials: Measurement, Quantification, and Visualization

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New and improved polymer materials are contributing to significant usable life and functional improvements of many products, contributing significantly to reduction of their lifetime environmental impacts. These enhanced materials typically utilize complex microstructures spanning multiple length scales that control their performance. In this context, it is important to simultaneously characterize wide range of length scales of these microstructures using nondestructive and quantitative tools. Combined Ultra-Small, Small, & Wide-Angle X-ray Scattering (http://usaxs.xray.aps.anl.gov) facility [1] at the APS has been serving soft matter community for over two decades. However, similar wide range instrumentation is available today from desktop SAXS manufacturers and, while slower, provides highly competitive data to synchrotron facilities [2].

With increased availability of high-quality extended range data to broad user community, easy and powerful data quantification and visualization tools are necessary. Advancements to time-tested Unified Fit model [3-5] extend understanding to the interpretation of analysis for this type of data and even enable visualization of representative microstructures. Irena [6] small-angle analysis package, since its January 2020 release, includes 3D aggregate model. This is Monte-Carlo method of generating 3D fractal aggregate structure (Figure 1) [7]. The original code was provided by Alex McGlasson from Beaucage group. This talk will discuss this and other new tools and capabilities in Irena and how are applied on hierarchical polymer filler structures and other advanced soft matter.

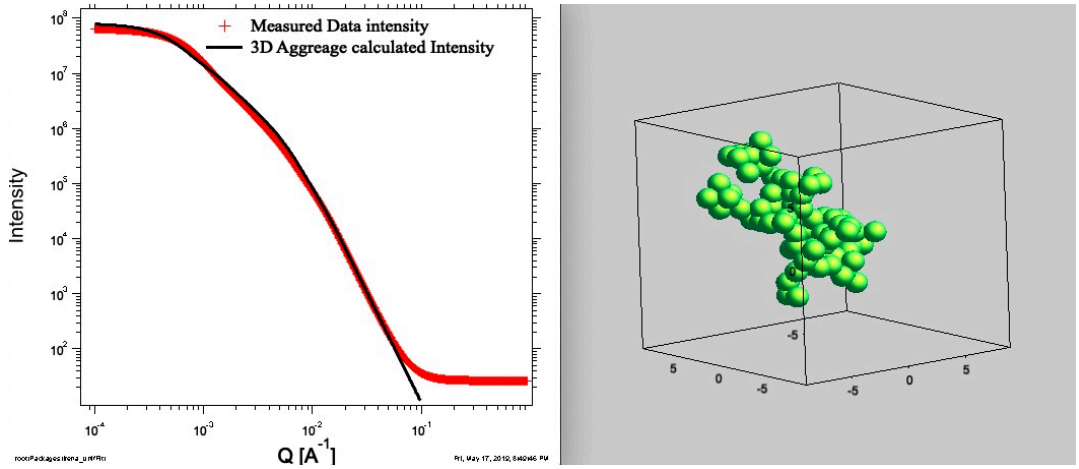

Figure 1. Left pane plots measured sample intensity and intensity calculated from the 3D aggregate particle generated using Monte-Carlo method. Right pane shows the 3D aggregate particle.

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