Development of a Simulation Driven Algorithm to Calculate Gold Nanorod Length Using Dynamic Light Scattering

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Gold nanorods were synthesized via the seed growth method and characterized with Dynamic Light Scattering (DLS) to create an algorithm to determine the distribution of their lengths. DLS measures the intensity of light after it is scattered from nanorod solution and determines the field correlation as a function of the natural logarithm of time. The most common method to calculate nanoparticle size from DLS data is the CONTIN method, which is complicated in the fact that it involves the decay rate of the scattered light intensity. In addition, CONTIN uses only apparent diffusion coefficient, which works best for spherical particles only. To improve on this method, Broserma's Hydrodynamic Equations were used to calculate the transverse and longitudinal diffusion coefficients and determine the field correlation function from the center-of-mass diffusion coefficient. By generating a simulation at uniformly distributed lengths and times, lasso regression was implemented to find the overall size distribution of the sample of nanorods. By comparing our results to the actual size distribution found using STEM and to results found using the CONTIN method, it was determined that the simulation-driven algorithm was more accurate at calculating the size distribution of the sample than the CONTIN method.