Real-time characterization of shape evolution of nanoparticles

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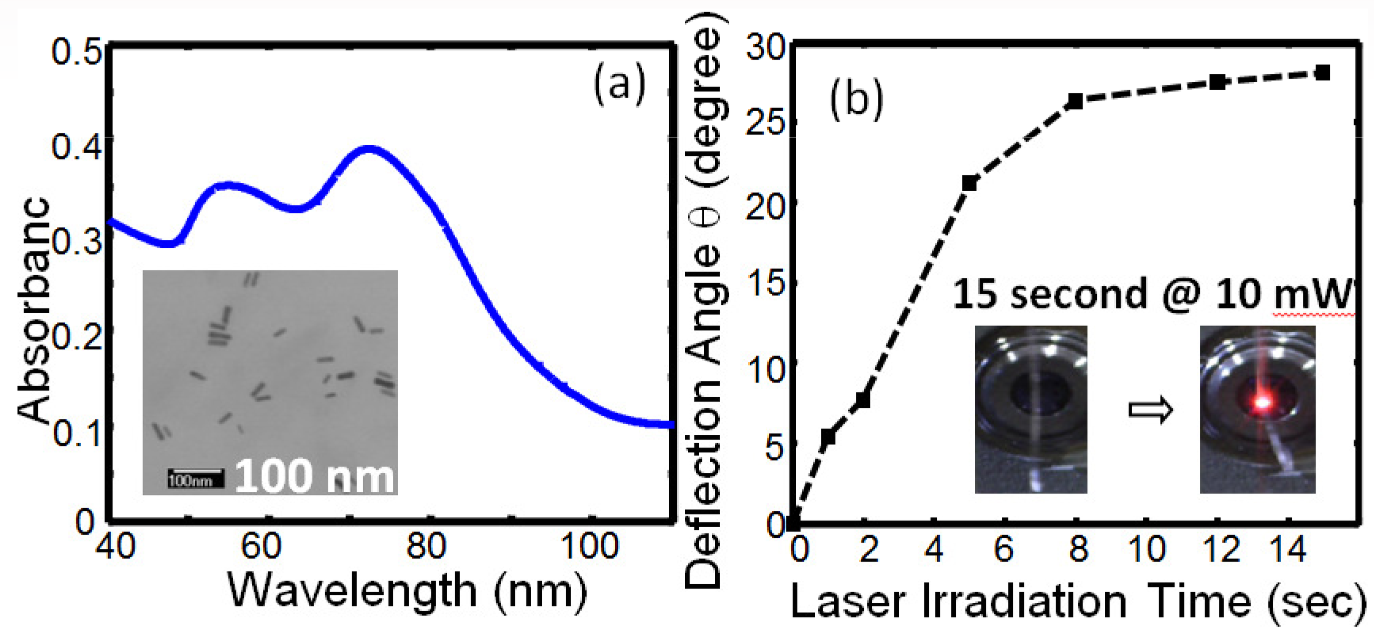
Motivation

- The plasmon resonance property of gold nanoparticles is promising for implementing a shape-change-triggering scheme in shape memory polymers, which have applications in self-healing structures, biomedical sensors, and switches.
- Producing gold nanoparticles with well-controlled shape and size is essential for obtaining the desirable plasmon resonance property.
- However, it has also been recognized that the current synthesis process is not robust. The quality (yield, size, and shape) is very sensitive to multiple factors. The lack of robustness for the current process has not been fully understood.

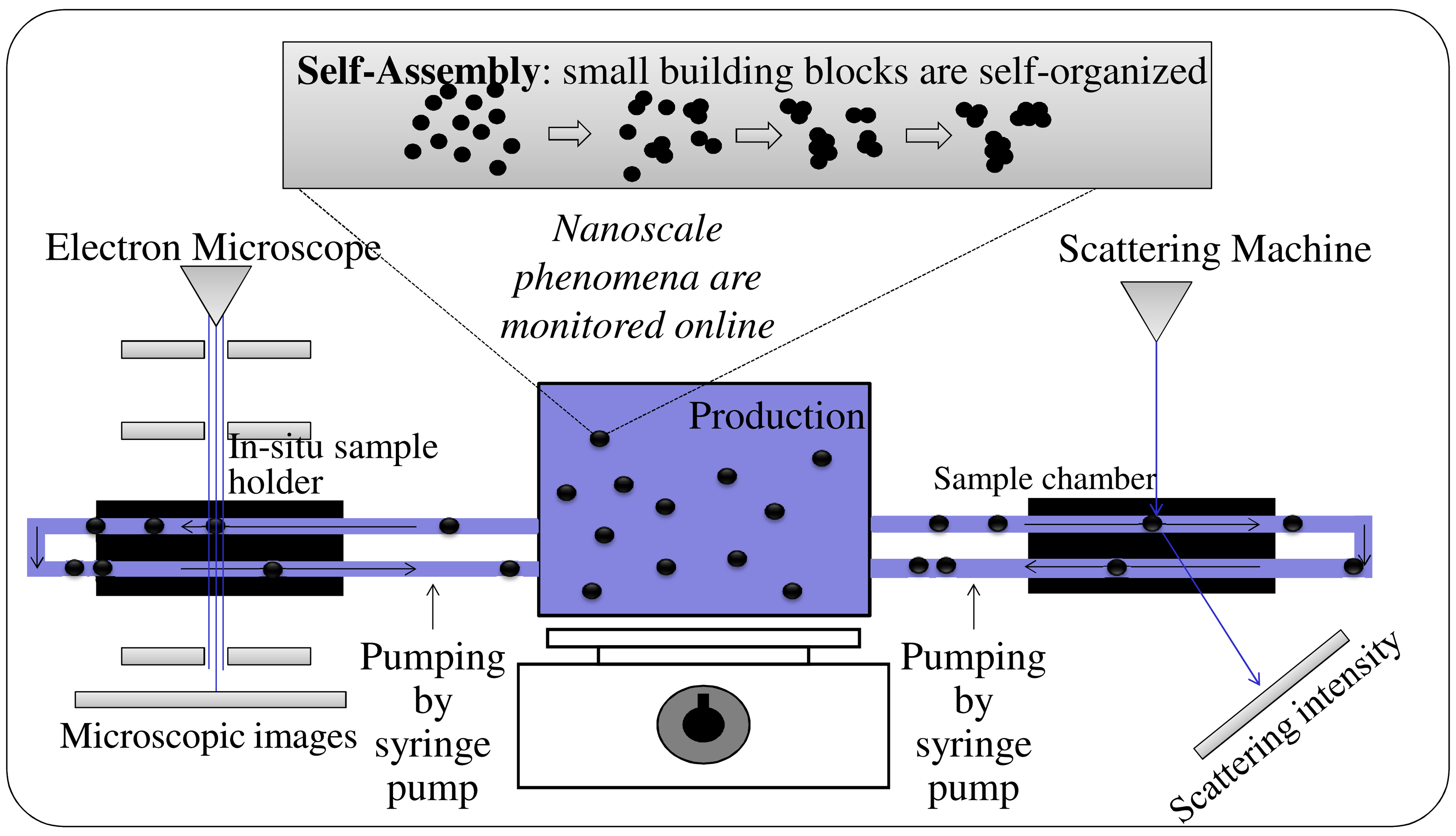


Objective:

The objective of the research is to study a predictive model to better understand the gold nanoparticle synthesis process in terms of nanoparticle's size and shape evolution, and use the predictive model as guidance for reliably producing and measuring gold nanoparticles with well controlled sizes and shapes.

Approach

- Analyze and improve a nanoparticle self-assembly process as a promising synthesis method.
- Use *in situ* measurement instruments (*in situ* microscopy and *in situ* scattering) to analyze high dynamic and stochastic nature of nanoparticle self-assembly processes.
- Combine two complementary *in situ* instruments to obtain process measurements at required length and time scales.
- Analyze the multi-instrument measurements together for more statistically robust estimates of particle sizes and shapes, and their temporal evolutions.

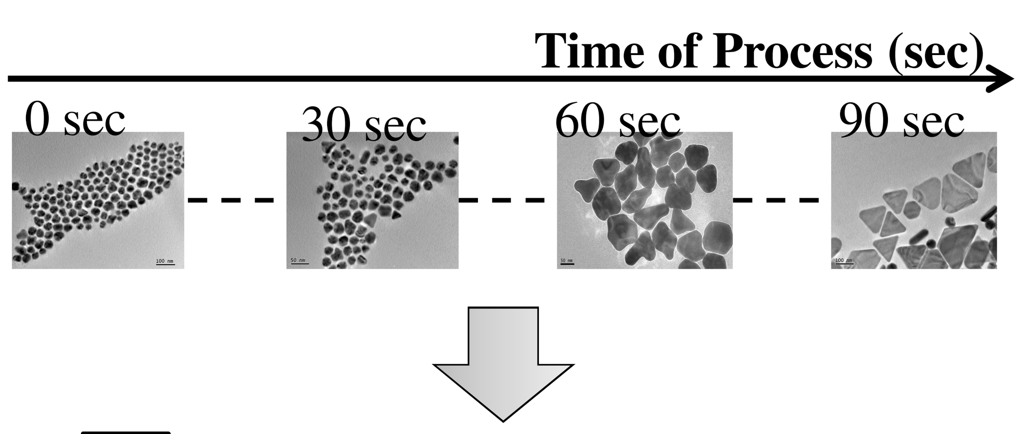


Accomplishment

T1: In situ TEM Data Analysis

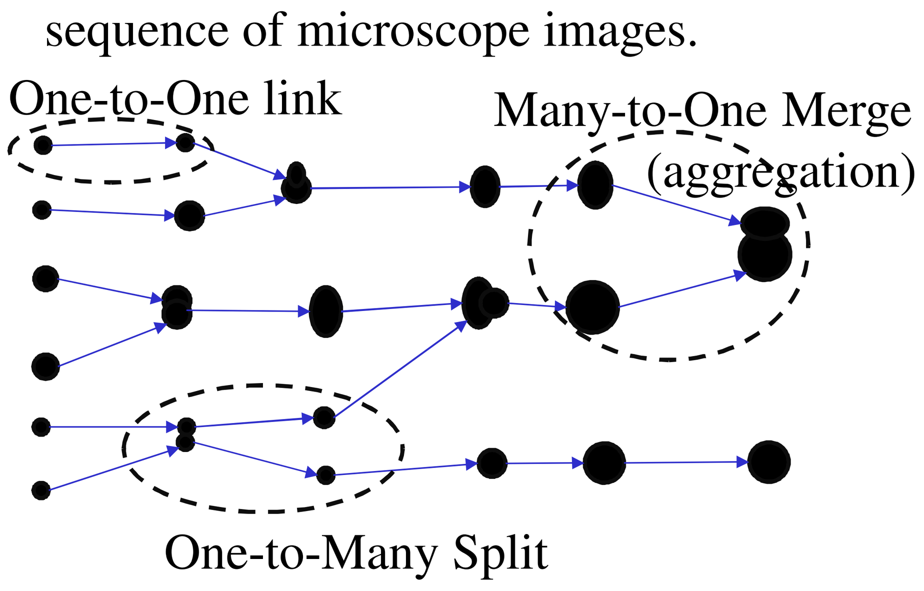
Sequence of Electron Microscopic Images

Temporally sparse but highly spatially resolving microscopic image data



A Realtime Nanoparticle Tracking

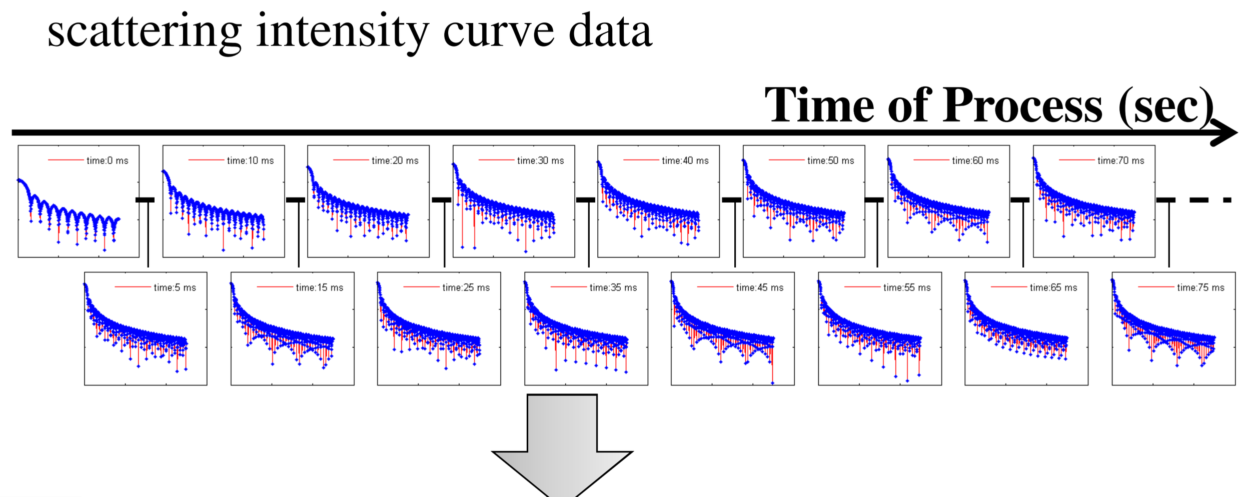
Track individual nanoparticles, their interactions, their shape evolutions in the sequence of microscope images.



T2 : In situ SAXS Data Analysis

Sequence of Scattering Intensity Curves

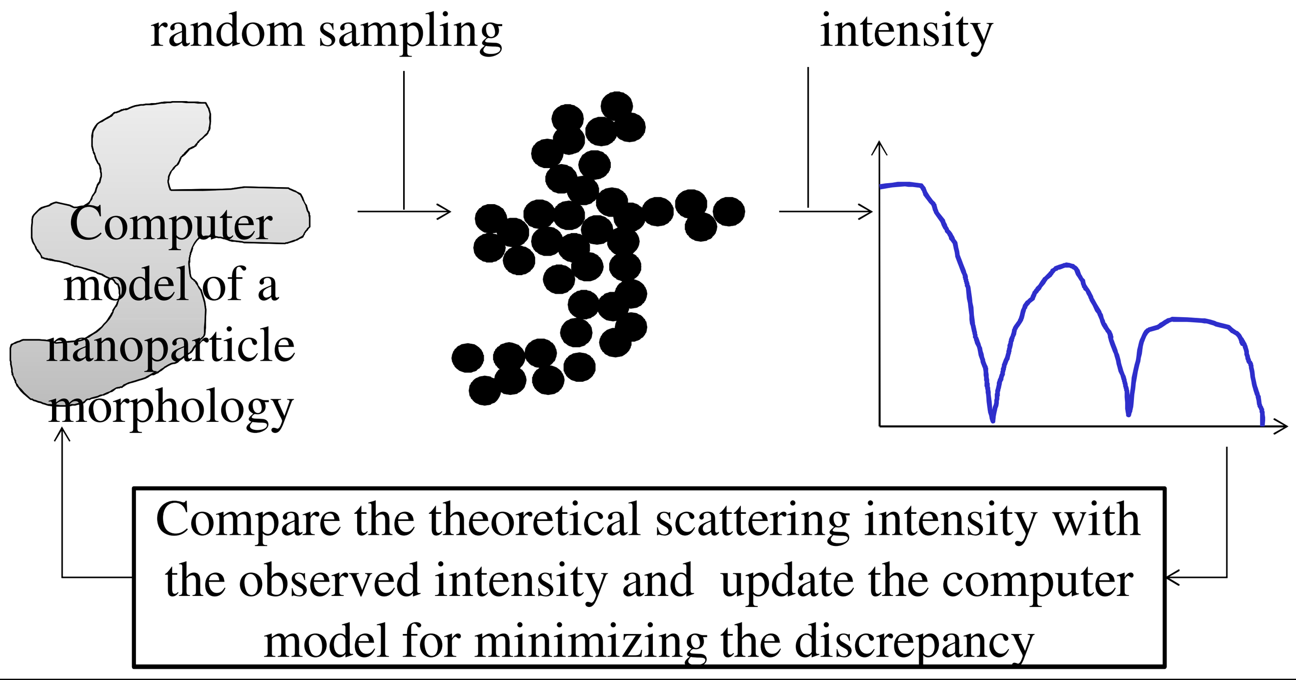
Spatially averaging but highly temporally resolving scattering intensity curve data



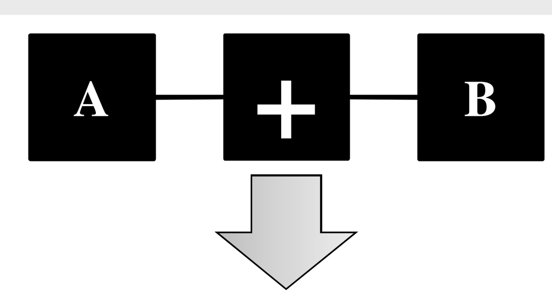
B Determination of Particle Mean Shapes Per Time

Generating n spheres within the structure by random sampling

Apply Debye's formula for theoretical scattering intensity

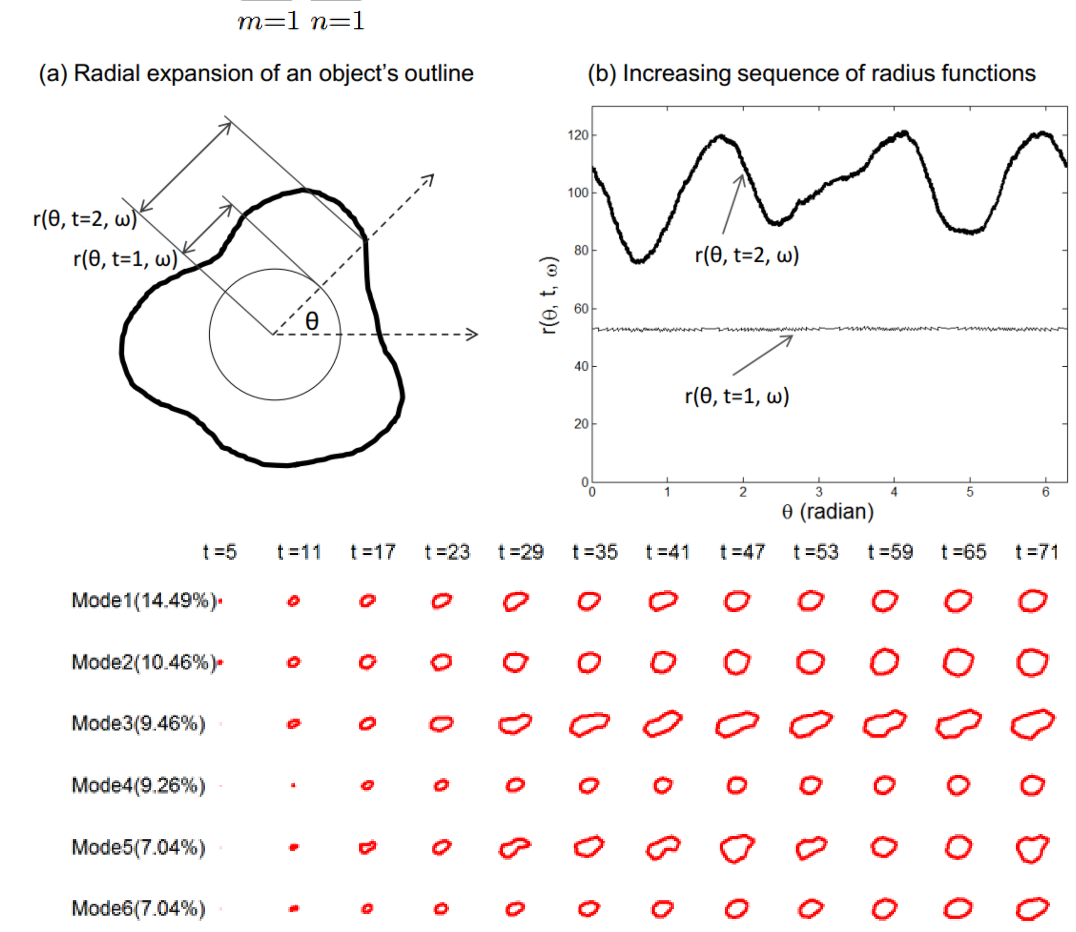


T3: Data Fusion of TEM and SAXS



Model and estimate a stochastic time series of a nanoparticle morphology evolution with microscopy data and scattering data

$$r(\theta,t,\omega)=\sum_{m=1}^{M}\sum_{n=1}^{N}\alpha_{m,n}(\omega)\phi_m(t)\gamma_n(\theta),\ t\geq 0 \text{ and } \theta\in[0,2\pi)$$



External Grants and Relevant Journal Articles

- Park, C. (PI), and Liu, T., *Dynamic Data-Driven Modeling of Nano Particle Self Assembly Processes*. AFOSR through Texas A&M University. (FA9550-13-1-0075). FSU portion $267,662.
- Park, C., Woehl, T. J., Evans, J. E., & Browning, N. D. (submitted). Minimum Cost Multi-way Data Association for Optimizing Large-scale Multitarget Tracking of Interacting Objects. *Journal of Machine Learning Research*. Manuscript submitted for publication, 1-24 pages.
- Park, C., & Shrivastava, A. (submitted). Multimode geometric profile monitoring with temporally correlated image data and its application to nanoparticle self-assembly processes. *Journal of Quality Technology*. Manuscript submitted for publication, 1-32 pages.
- Park, C. (tentatively accepted). Estimating multiple pathways of object growth using non-longitudinal image data. *Technometrics*, 1-26 pages.

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