2017 ChemMatCARS Summer Student Program Report

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This is a brief account of my stay at the Advanced Photon Source (APS) at Argonne National Laboratory (ANL) from May 8th through June 9, 2017 as part of the Student Development Program currently being awarded to graduate students to introduce them to the current state of the art ChemMatCARS facilities at Argonne National Laboratory.

I am a Chemical Engineering PhD student from the University of Illinois at Chicago. I am studying the ordering of passivated gold nanoparticles at an electrified liquid/liquid interface. My goal is to use x-ray scattering to probe ordered structures of gold nanoparticles at an electrified interface of water and oil. I want to understand the interactions responsible for nanoparticle position, transport and ordering at the interface. I use electro-chemistry techniques, mainly potentiostatic, potentiodynamic, and cyclic voltammetry together with the complimentary techniques of quasi-elastic light scattering, x-ray reflectivity and GISAXS techniques to address my goal.

I have been a regular user of the Advanced Photon Source (APS) at Sector 15 for the past 6 years under the supervision of Prof. Mark Schlossman whose Laboratory at the University of Illinois at Chicago focuses on different aspects of interfacial studies of which my study is on the ordering of passivated gold nanoparticles at the water/oil interface. Other students, both past and present whom I work with also specialized in areas such as solvent extraction of heavy metal ions at water oil interface, gold reduction at water/oil interface and anomalous study of metal ions at a liquid/liquid interface. I was involved in most of these projects which also used the APS facility to understand the structure at the interface. Analyzing this data requires an extensive understanding of x-ray interactions with matter and special programming skills.

During my 4 week stay at ChemMatCARS I was directly supervised by Mrinal Kanti Bera and Wei Bu who are beamline scientists at ChemMatCARS. They

engaged me on day to day basis and monitored my progress. Binhua Lin, the Senior Scientist at ChemMatCARS, Sector 15 was also actively involved throughout my stay and constantly monitored my progress and well-being as well. Binhua Lin gave me the opportunity to come and learn here. Not to forget Yu-Sheng Chen and Mati Meron who always inspired me and encouraged me throughout my stay.

I consider myself fortunate to have been given the opportunity to learn from the very talented and committed scientists at ChemMatCARS Sector 15. The staff from ChemMatCARS guided me through data processing of x-ray measurements to modeling the data in order to extract important structural information from the ordered system of gold/water/oil. I will describe this incredible experience and how together with the help of ChemMatCARS staff at Sector 15, I managed to successfully achieve my goal.

My main task was to analyze x-ray experimental data of passivated gold nanoparticles ordered at an electrified water/oil interface. This is part of my on-going PhD thesis work. I am interested in understanding the interfacial ordering of the nanoparticles, including their packing, in terms of domains, coverage, size, and position at the electric water/oil interface. Understanding how these nanoparticles transport and order at the interface can address several industrial and scientific problems. They also have important industrial applications to which my understanding can optimize their applications.

My first journey in data analysis was a qualitative analysis of the experimental data to get a sense of direction in order to create meaningful and physical mathematical functions describing the experimental data.

Next was the quantitative analysis, which involved a detailed mathematical description of the qualitative information from my data. I used the python programming language to write different modules of mathematical functions describing the interfacial dynamics of my system. This was the model development stage. After developing models, we tested their integrity using the principles and theories of x-ray reflectivity in addition to

intuition and experience. It is always important to have confidence in the model by rigorously testing it with fundamental theories, intuition and experience.

Having established confidence in our model, we did model sensitivity analysis. This was done by testing and understanding the role and effect of each model parameter under consideration as well as their relationship or correlation with each other.

After the sensitivity analysis, we proceeded to fitting our experimental data. Fitting the data now became easier because I had acquainted myself with the model and obtained a sense of the role of the fitting parameters.

Finally, we did an error analysis on our fitted data to test the accuracy of each extracted unknown parameter from our model. This also has to undergo rigorous logical analysis, intuition and confidence based on unbiased critical thinking. As the great statistician, George Box once said, "All models are wrong but some are useful". For this reason, several other different models were proposed and tested against our original model. Some are currently under consideration and are being tested to justify the uniqueness of our model and its ability to accurately describe our system of water/oil/gold nanoparticles system with the least error and uncertainty.

In the course of my learning, I frequently talked with my Advisor, Prof. Mark Schlossman for his opinions, suggestions and guidance as well. He also visited me at ChemMatCARS to ensure that I was doing well.

What is so fascinating and exciting about this Student Development Program is the structure and competence of the staff of ChemMatCARS sector 15. They walk you through daily tasks and give you honest feedback. My time here has been awesome. The atmosphere at ChemMatCARS inspired me to push beyond my ability. Here there is nothing like an "I can't do it" mentality. The way the staff relentlessly address challenges is very inspiring and I hope to build on this experience in my career.

Overall, I learned a lot. Adding the experimental skills that I have acquired over the years at APS sector 15 to the analytical approach of analyzing data I have just acquired, to me, is a complete way of developing as a young scientist and engineer. I hope to build on the set of skills, knowledge and experience that I have acquired at ChemMatCARS to contribute to the scientific and engineering communities.

My study here has been great because of the help of the hardworking staff at ChemMatCARS whose patience and warmth made my stay here wonderful. Special thanks goes to all the staff of Sector 15 ID, but especially to Mrinal Kanti Bera, Wei Bu, Binhua Lin, Yu-Sheng Chen, Kimberly Simms and Mati Meron. I also had a great time working and spending time with other graduate students who are also receiving training in different areas. Special thanks goes to these graduate students, Peiyou Quan, Seiji Katakura, and Tieyan Chang. I am grateful for the opportunity given to me by ChemMatCARS under the auspices of the University of Chicago for this experience. I look forward to the future with renewed optimism and confidence after this great experience. Thank you.

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