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X-ray Studies of Nano Composites¹ ALEXANDER HEXEMER, LBNL

Nano composite materials are an exciting and fast expanding field. X-ray scattering has been used in order to study the structure properties relation. During the last few years the field has expanded more towards the field of thin films where theres been a dramatic increase in the use of grazing incidence small angle X-ray scattering (GISAXS). The main issue of GISAXS has been the complex analysis framework necessary for simulating and fitting. In addition, existing software has restricted the scientist in systems that can be simulated and the speed to analyze large amounts of data. Over the last few years we have worked closely with our computational research and supercomputer division to enable the use of supercomputers to simulate at scattering data. We have developed a comprehensive analysis framework to simulate and fit a wide variety of materials and morphologies. The framework is designed to supply scientists with close to real-time feedback during beam times. Therefore, HipGISAXS (High Performance GISAXS) has been developed to run simulations on massively parallel platforms such as the Oak Ridge Supercomputer Titan (OLCF). Further, with inverse modeling algorithms for fitting available in HipGISAXS, such as particle swarm optimization, it can handle a large number of parameters during the structure fitting process. In September of 2014, HipGISAXS was used in a real time demonstration that married the SAXS/WAXS beamline at the ALS with the data handling and processing capabilities at NERSC, and simulation capabilities of running at-scale simulations on Titan at OLCF.

¹DOE Early Carrier Award, SPOT and CAMERA