High-Performance GISAXS Code for Polymer Science*

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Grazing Incidence Small-Angle Scattering (GISAXS) is a valuable experimental technique in probing nanostructures of relevance to polymer science [1]. Experimentalists are expressing a growing need for efficient and scalable simulation tools to dissect the massive volume of GISAXS data gathered at state-of-the-art beamlines. New high-performance computing algorithms, codes, and software tools have been developed to analyze GISAXS images generated at synchrotron light sources.

We have implemented a flexible GISAXS simulation code based on the Distorted Wave Born Approximation (DWBA) written in C++/CUDA to run on a GPU cluster [2]. The software computes the diffraction pattern for any given superposition of custom shapes or morphologies (e.g. obtained graphically via a discretization scheme) in a user-defined region of the reciprocal space for all possible grazing incidence angles and sample rotations. This flexibility allows a straightforward study of a wide variety of possible polymer topologies and assemblies whether embedded in a thin film or a multilayered structure. Hence, this code enables guided investigations of the morphological and dynamical properties tied to photovoltaic materials, carbon capture and sequestration technologies, fuel cell devices and other applications in polymers science.

The current parallel GPU code is capable of computing GISAXS images for highly complex structures and with higher resolutions and attaining speedups of over 200x compared to the sequential code [3]. An example of such computation is given in Figure 1.

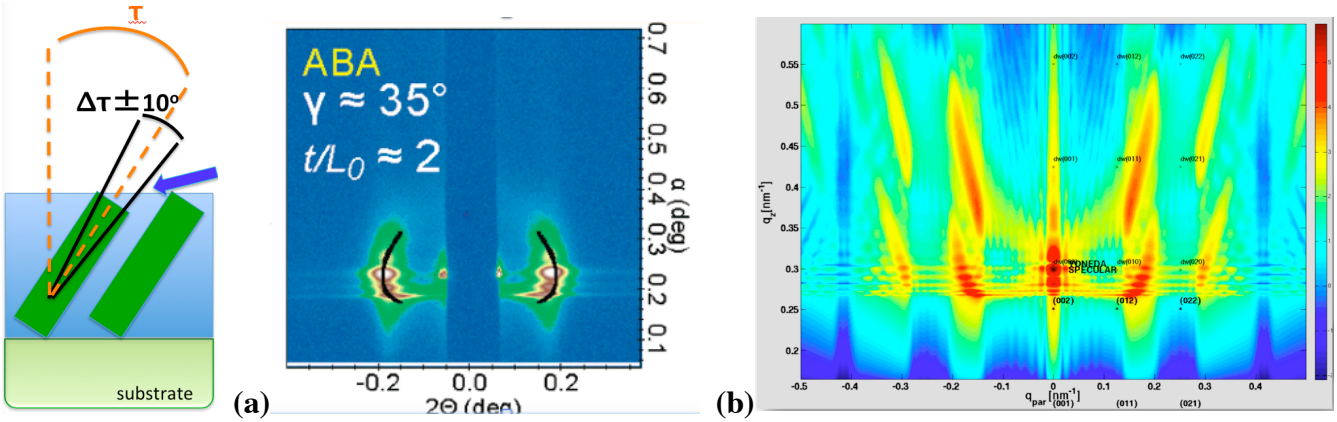

Figure 1: Experimental [4] (a) and computed (b) GISAXS images of a triblock copolymer (ABA) with tilted domains at 35°±10° at incidence above the critical angle. The averaging of the lamellar tilt angle recovers the curved feature indicated by solid black lines in (a).

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References

[1] Gilles Renaud, Rémi Lazzari and Frédéric Leroy, Surface Science Reports **64** (2009) 258–263;

[2] S. T. Chourou, A. Sarje, X. Li, E. Chan and A. Hexemer, "GISAXS Simulation and Analysis on GPU Clusters", *MAR12 Meeting of the American Physical Society*, Session B45.00014;

[3] A. Sarje, J. Pien, X. Li, "GPU Clusters for Large-Scale Analysis of X-ray Scattering Data", submitted to *NVIDIA GPU Technology Conference*, May 2012;

[4] G. E. Stein et *al.* Macromolecules Vol. **41**, No. 7 (2010).