Topological Validation of Morphology Modeling by Reverse Monte Carlo Analysis of Two-dimensional Scattering Patterns KATSUMI HAGITA, National Defense Academy, JAPAN, TAKASHI TERAMOTO, Chitose Institute of Science and Technology — We presented a new method of morphology modeling using coarse- grained particles from multiple two-dimensional (2D) patterns of structure factors, which can be obtained from small angle x- ray scattering (SAXS). Reverse Monte Carlo (RMC) technique is extended for multiple 2D patterns. It is motivated by SAXS experiments of kinetic pathway from hexagonal perforated lamellar structure to double gyroid (DG) structure in the surfactant/water systems. For the first test, we examine reproducibility of a DG morphology. As a reference configuration, we obtain positions of particles forming DG morphology are generated in a computer using the equation of DGs surface. Inputs of this extended RMC method are calculated from this reference configuration. The configurations obtained from this extended RMC method are examined by the Betti numbers which are mathematical indexes to classify complicated inter- connected three-dimensional structures and are given by Computational homology (CHomP) analysis. Combination of RMC and CHomP is examined as a new and useful approach for connecting scattering experiments to mathematics for 3D morphology.

Katsumi Hagita
National Defense Academy, JAPAN