SAXS Studies of Nucleation of Glycine from its Supersaturated Solution

Soma Chattopadhyay^{1,2}, Deniz Erdemir², James M.B. Evans³, Jan Ilavsky⁴, Heinz Amenitsch⁵, Carlo U. Segre^{1,6}, Allan S. Myerson², ¹MR-CAT, Advanced Photon Source, Building 433B, Sector 10, Argonne National Laboratory,9700 South Cass Avenue, Argonne, Illinois 60439, USA. ²Department of Chemical and Environmental Engineering, Illinois Institute of Technology, Chicago, Illinois 60616, USA. ³Glaxo Wellcome Manufacturing Pte Ltd., 1 Pioneer Sector 1, Singapore, 628413. ⁴Argonne National Laboratory, Building 438 E, APS, 9700 South Cass Avenue, Argonne, Illinois 60439, USA. ⁵Institute of Biophysics and X-ray Structure Research, Austrian Academy of Sciences, Schmiedlstrasse 6, A8042, Graz, Austria. ⁶Department of Biological, Chemical and Physical Sciences, Illinois Institute of Technology, Chicago, IL 60616, USA. E-mail: soma@agni.phys.iit.edu

The early stages of the process of crystallization, especially that of small molecules from their supersaturated solution is not yet fully understood. In an effort to understand the process of nucleation and crystallization of such molecules, small angle x-ray scattering (SAXS) has been used to study the crystallization of the amino acid glycine from its supersaturated aqueous solution. The scattering data was analyzed using the Unified Fit Model which helps in studying complex systems that may contain multiple levels of related structural features. The results suggest that glycine molecules exist as dimers in supersaturated solution. The structure factor and the form factor obey power-law behaviour that indicates the presence of fractals in the solution. A transformation from mass fractal structure to surface fractal structure is observed during the crystallization process.

Keywords: SAXS, nucleation, fractals