

Topological investigation of electronic silicon nanoparticulate aggregates using ultra-small-angle X-ray scattering

Jonah, EO¹, Britton, DT¹, Beaucage, P², Rai, DK², Beaucage, G², Magunje, B¹, Ilavsky, J³, Scriba, MR^{1,4}, and Harting, M¹

¹*Department of Physics, NanoSciences Innovation Centre, University of Cape Town, Rondebosch 7701, South Africa*

²*Department of Chemical and Materials Engineering, University of Cincinnati, Cincinnati*

³*X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439, USA*

⁴*CSIR. Materials Science and Manufacturing*

Abstract

The network topology of two types of silicon nanoparticles, produced by high energy milling and pyrolysis of silane, in layers deposited from inks on permeable and impermeable substrates has been quantitatively characterized using ultra-small-angle X-ray scattering, supported by scanning electron microscopy observations. The milled particles with a highly polydisperse size distribution form agglomerates, which in turn cluster to form larger aggregates with a very high degree of aggregation. Smaller nanoparticles with less polydisperse size distribution synthesized by thermal catalytic pyrolysis of silane form small open clusters. The Sauter mean diameters of the primary particles of the two types of nanoparticles were obtained from USAXS particle volume to surface ratio, with values of ~41 and ~21 nm obtained for the high energy milled and pyrolysis samples, respectively. Assuming a log-normal distribution of the particles, the geometric standard deviation of the particles was calculated to be ~1.48 for all the samples, using parameters derived from the unified fit to the USAXS data. The flow properties of the inks and substrate combination lead to quantitative changes in the mean particle separation, with slowly curing systems with good capillary flow resulting in denser networks with smaller aggregates and better contact between particles.