Contribution ID : **289** Type : **Poster**

Using Synchrotrons to unravel the Chemistry of Nucleation

The formation and growth of nanoparticles is of critical importance in a variety of scientific areas and in everyday life. The prevailing models used to describe these processes have mainly been based on thermodynamic arguments and by the use of concepts such as “monomers” or “particles”, thereby omitting to incorporate the important influence of differences in the chemical nature of different systems. One of the main reasons for this lack of incorporation of the chemistry into these models has been the lack of quantitative information on an atomistic level obtained in situ during nanoparticle formation, i.e., characterization methods that enable the extraction of atomic level structural information, preferably at a suitable time resolution under real experimental conditions.
I will present an overview numerous in situ studies we have performed using numerous different tools that enable extraction of atomistic structural information about the formation and growth of nanoparticles during Sovothermal synthesis. The main characterization methods have been synchrotron based in and ex situ PXRD, total X-ray scattering, PDF-analysis and EXAFS. The data has been analyzed by sequential Rietveld refinement, real space Rietveld refinement, curve fitting, Debye scattering equation based techniques and other methods. Our studies have revealed a fascinating chemical richness spanning from mono-metal to complex polymer precursor species, which through a specific system-dependent multistep mechanism develop into pristine nanomaterials.
The results have led us to call for a paradigm shift in how nucleation of nanoparticles is conceived – it is imperative to move away from a one-fits-all approach and instead consider many-fit-many models that incorporate the true chemistry of different systems, rooted in atomistic chemical insight obtainable to a large degree by the use of Synchrotron radiation.

Reference: The chemistry of nucleation, Bøjesen et al. CrystEngComm, 2016,18, 8332-8353

Keywords or phrases (comma separated)

In situ, PDF, Total scattering, Nucleation

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Track Classification : Advanced Materials