Nanostructure analysis in real space: PDF studies of nanoparticle chemistry

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Nanomaterials have come to play a huge role in modern materials chemistry: By nanosizing the functional materials used for a range of applications, e.g. batteries and catalysis, many properties can be improved. This development has challenged our understanding of structure/property relations, as the conventional techniques for material characterization break down for structures on the nanoscale. However, total scattering combined with Pair Distribution Function analysis allows us to look further into nanostructure and establish this relation for many advanced functional materials,[1] opening a whole new level of insight for material chemists.

Here, I will present recent work illustrating how we use total scattering to characterize nanomaterial structure and show how Pair Distribution Function analysis can be used to elucidate the atomic arrangements in even the tiniest of nanoparticles and nanoclusters, with special focus on metal and metal oxide nanoparticles.[2,3] Using PDF, we observe that new structural motifs, unstable in the bulk form, become dominant in nanoscale materials. In gold clusters, for example, we use PDF analysis to determine the atomic arrangement in 2 nm particles, where *fcc* structures are no longer stable.[2] In oxide materials, we see that defects know from bulk materials completely dominate the atomic structure on the nanoscale, and changes the atomic arrangement significantly, highly affecting their properties.[3] We also apply total scattering techniques to gain a new understanding of the reactions and processes taking place during crystallization of materials. In situ PDF methods allow following structural changes throughout a synthesis, all the way from an ionic cluster in solution, over amorphous intermediates and to the final crystalline material, making it possible to gain new insight into nucleation mechanisms.[5] I will furthermore show how total scattering combined with computed tomography can open for a range of new *in situ* studies, as nanostructure can now be positionally resolved.

References

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