Accelerated materials discovery through in situ X-ray diffraction

Bo Brummerstedt Iversen

Center for Sustainable Energy Materials, Department of Chemistry, Aarhus University, Denmark

bo@chem.au.dk

Humankind depends on the continuous development of new materials, but the long period from discovery to application constitutes a substantial challenge. Currently, there is a strong focus on establishing automated synthesis laboratories, where artificial intelligence can discover and optimize synthesis pathways. Presumably robots can perform the synthesis, while machine learning is used in feedback loops based on on-line data from various analytical measurements. However, so far, the synthesis methods used in AI-assisted automatization are very simple and this limits the available materials and prohibits complex atomistic design.

Two decades ago, we introduced in situ PXRD studies of solvothermal reactions to enhance our fundamental understanding of crystal formation. During the past decade these studies have been expanded to include in situ PDF analysis, and in situ solvothermal reactors are now available for general use e.g. at PETRA3 and Max IV. In situ PXRD and PDF studies provide a direct probe of the synthesis process while it takes place, and a typical synchrotron beamtime of 3-4 days corresponds to empirical testing of thousands of sequential ex situ synthesis experiments in the laboratory. This means that optimal synthesis conditions can quickly be uncovered. Additionally, the formation of potentially metastable phases absent in the final product, or the occurrence of complex multistep reaction pathways, is unveiled.

Based on 10 years of in situ studies we were able to develop a simple efficient solvothermal synthesis route for complex solid solution metal alloy nanoparticles, and we are now exploring the vast composition space provided by this method. In this talk I will discuss recent results on binary alloys as well as investigations of entropy effects on the electrocatalytic properties of nanoparticle catalysts.