Simulation study of superheating in evaporating droplets in spray flame synthesis of battery materials

Babette Kunstmann, Hans Hasse, Maximilian Kohns

Spray flame synthesis is a promising gas-phase technique that can e.g. be used for the production of battery materials. One example is nanoscale spinel lithium titanate ($Li_4Ti_5O_{12}$, LTO), which is an anode material for lithium-ion batteries with high life cycle capabilities. Low particle sizes and surface modifications, which can both be achieved by tuning the parameters of the spray flame synthesis process, improve the electrochemical performance of LTO-based anodes.

In spray flame synthesis, high quality product nanoparticles are usually only obtained when droplet micro-explosions droplets occur during the process. There is an ongoing debate on the causes of these micro-explosions. With the present simulation study, we contribute to the clarification of this issue. As an example, we study mixtures of titanium (IV) isopropoxide (TTIP) + *p*-xylene, which are a common constituent of LTO precursors.

To this end, a one-dimensional model is developed, in which both the energy transport and the mass transport inside the droplet and the corresponding convective boundary conditions are considered. From the temperature and concentration profiles in the droplet, the superheating is calculated, considering the non-ideality of the liquid phase. The results show that superheating sets in inside the droplet. Hence, after reaching a certain threshold, a sudden evaporation will occur inside the droplet – and cause the micro-explosion. This effect is related to large values of the Lewis number, indicating that the heat conduction is much faster than the mass diffusion. As the Lewis number is not only large for the system studied here but also for other precursor solutions used in spray flame synthesis, the explanation of the observed micro-explosions is expected to hold in many cases.