Laboratory for advanced structural studies (LASS):

In addition to the study of atomic structures, our research focuses on the investigation of hierarchically organized structures at the nano- and mesoscopic scales. Our research activities are wide-ranging and include the study of various nanostructures and their hybrid systems, lead iodide–based perovskites, as well as doped diamond samples. Through theoretical calculations, we model the formation of eutectic alloys.

Stable perovskite–nanotube hybrid nanostructures

Perovskite-filled nanotube systems represent a particularly promising class of hybrid nanostructures. Nanoscale encapsulation enables the exploration of confinement-induced effects on optical properties, while the nanotube host provides protection against environmental degradation, addressing one of the key limitations of perovskite-based materials.

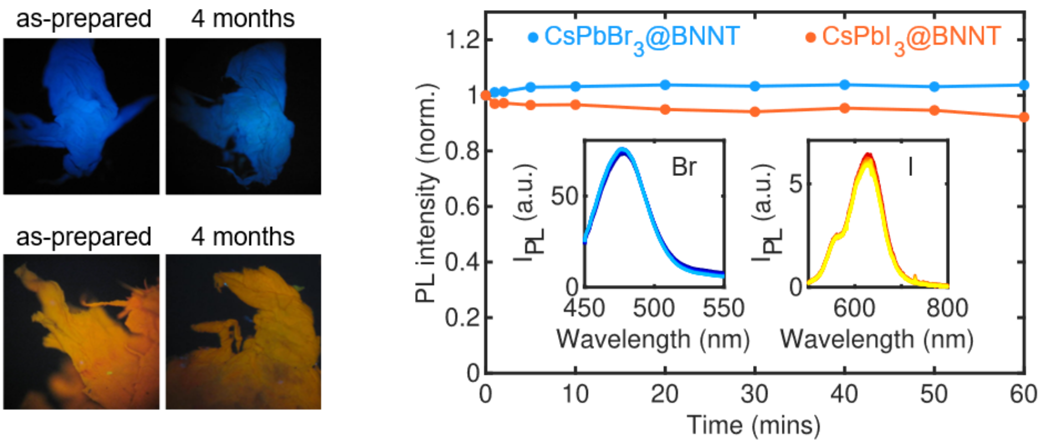

Figure 1. Demonstration of the stability of the samples. Left: Photos under 380 nm UV illumination of the CsPbBr3@BNNT (blue) and CsPbI3@BNNT samples (yellow). Right: Photoluminescence of the encapsulated quantum wires.

This year, we worked out the synthesis of emissive perovskite quantum wires with high aspect ratio and narrow diameter, encapsulated within boron nitride nanotubes. Owing to the wide bandgap, and, consequently, wide transparency window of boron nitride nanotubes, the photoluminescence of the confined perovskite nanowires is directly accessible, in contrast to carbon nanotube–based heterostructures. This system represents the first demonstration of a luminescent heterostructure formed by an inorganic crystalline material inside a boron nitride nanotube, with optical properties critically governed by nanoscale confinement. The resulting hybrid nanostructures combine optical tunability, linearly polarized emission, and enhanced stability (fig. 1.), highlighting their significance as model systems for fundamental optical studies and as building blocks for future nanophotonic and optoelectronic devices. The corresponding results are currently submitted for publication.

Mapping ion damage and NV formation in diamond

In close cooperation with the ATOMKI institute in Debrecen, we fabricated well-defined parallel graphitized channels in single crystal diamond. Using 1.3 MeV and 2 MeV proton beams we designed two layers with confined damaged regions in the nitrogen doped crystal, where upon high temperature annealing we were able to create high density ensembles nitrogen-vacancy (NV) centers. By varying the proton beam fluence, each region experienced different lattice damage which primarily influenced vacancy formation yield and consequently the final NV center concentration and charge state ratio of the two subtypes of NV centers i.e the negatively charged and charge neutral types. Using Raman scattering spectroscopy we identified the fluence limit to avoid permanent damage to the lattice that cannot be recovered upon high temperature annealing, while Raman and fluorescence imaging gave us insight into the fluence dependent NV formation yields. Raman scattering spectroscopy reveals the energy dependent stopping range of ions in the crystal. This result agrees well with our SRIM simulations showing that the hyperspectral Raman imaging is a capable tool to determine ion penetration depth. Fluorescence imaging showed that the vacancy diffusion length is limited as the NV center intense regions correlate with vacancy rich regions prior annealing.

Eutectic melting of 3D rod structures

In collaboration with colleagues from the University of Michigan (US), we started a study on the melting of a directionally solidified rod-type Al-Al_3Ni eutectic structure. Using the in-situ synchrotron data the colleagues obtained, we used the real 3D structure as initial condition of our simulations. By quantitative phase-field modeling we can not only simulate the melting process and compare it to the experiment but also vary the process and materials parameters to learn more about the system. We have investigated how the lead distance (the height of the rods with respect to the eutectic surface) depends on the rod-rod distance, the local phase fraction and the melting speed. In our simulations, we successfully reproduced the spherodization (the detachment of small spherical solid particles from the end of the melting rods) observed in the x-ray images (Figure 2).

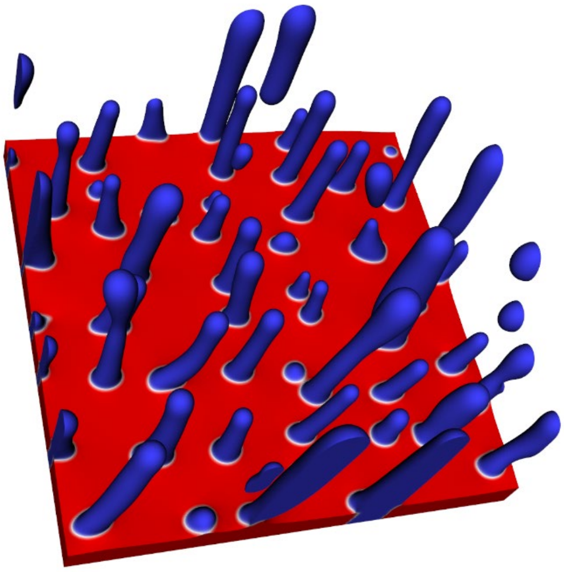

Figure 2. Directional melting of an Al-Al_3Ni eutectic structure obtained by phase-field simulation using the experimental X-ray tomography 3D data as input. At the nominal composition, the Al_3Ni solid phase (blue) has a significantly higher liquidus temperature than the Al solid phase (red), thereby the rods emerge from the eutectic surface. Numerous spherodization events can be observed, where a small spherical particle is detaching from the end of its rod.