Towards the development of novel functional nanomaterials: Establishing processing-structure-property relationships in single nanoparticles of binary alloys

Inorganic nanoparticles with a size less than 100 nm represent a new class of materials. They exhibit extraordinary physical, chemical, and electronic properties, which are size-dependent. As a result, the current and potential applications for nanoparticles are constantly growing, covering a broad range of materials for health, energy, transport, and information and communications technology. For example, they are used in magnetic resonance and thermal imaging, sensing, drug delivery, biomedicine, electronics, catalysis, magnetic data storage, plasmonic, optoelectronic, and thermoelectric devices.

Over the last decades, two-component nanoparticles have attracted attention of scientists. The presence of two different chemical elements in nanoparticles offers an additional degree of freedom for tailoring their physical and chemical properties. It is the atomic mixing pattern, which describes the arrangement of atoms within the nanoparticle. The atoms may be randomly mixed, forming a homogeneous structure, or they may form a Janus-like nanoparticle with two parts comprising different elements. A core-shell structure is one more option. Some patterns are formed spontaneously in nanoparticles, while the others are designed artificially and could exist in a limited temperature range, i.e. they are metastable. The metastable phases and mixing patterns are of particular interest as they provide new functionalities by accessing material properties beyond those of equilibrium ones. Thus, mixing of unmixable chemical elements in a single nanoparticle, scientists fabricate materials, which do not exist in nature and benefit from emerging properties. For example, semiconductor nanoparticles doped well beyond the equilibrium concentrations exhibit optical properties of noble metals. Another strategy is combining two disparate materials onto a single Janus-like nanosystem, thus providing multiple functionalities stemming from the unusual materials combinations. For example, by combining magnetic Co, Ni, or Fe with plasmonic Au, Ag, or Cu in a single nanoparticle, scientists design a multifunctional material exhibiting simultaneously optical and magnetic phenomena. Such nanoparticles are often referred as to hybrid nanomaterials.

At the same time, understanding processes governing the formation of atomic mixing patterns in two-component nanoparticles remains a grand challenge for nanophysics and nanotechnology. This is because of a finite volume of a nanoparticle, which is game-changing. The physical rules, which are universally applied to bulk materials, often fail at the nanometer scale, while the new ones are unexplored yet. Therefore, in this project, we aimed to tackle this problem and to establish the mechanisms of formation and separation of phases in two-component nanoparticles under solid↔liquid and solid-solid transitions. The second goal is to explore the effect of mixing patterns on the physical properties of nanoparticles.

We will use Au-Ge, Ag-Cu, Sn-Ge, and Au-Ni nanoparticles with the size varied in the range of 5 - 200 nm. The nanoparticles will be thermally cycled directly in a high-resolution transmission electron microscopy (TEM) using a novel heating holder. We expect to see how the atoms are arranged within the nanoparticles at different temperatures, how a nucleus of a new phase forms and grows. These observations enable us to identify the pathways of separation of phases in two-component nanoparticles. With this knowledge, we will be able to manipulate the nucleation mechanism and fabricate equilibrium and metastable mixing patterns in nanoparticles. Furthermore, we will probe the optical and thermal properties of the fabricated nanoparticles using cutting-edge TEM and atomic force microscopy (AFM) techniques. The synergetic combination of these techniques for characterization of the very same nanoparticle will leverage the quality and amount of the collected data to an unprecedented level. As a result, the processing-structure-property relationships will be established for single nanoparticles.