Diffusion in bimetallic nanoalloys.

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Objectives: It was proved experimentally that the dominant mechanism of diffusion in metals is via vacancies - not occupied nodes of crystalline lattice. This is why in alloys various metals at high temperature can migrate with different rate forming sometimes colorful moving interface between slabs of metals. Former ideas of ring-like lattice atom exchange could not stand the test of experimental evidence. In nanocrystalline material however, its large surface is often exposed to chemical interactions which may affect vacancy formation as well as surface segregation phenomena. The latter is a diffusion thermodynamic process satisfying preference of some metals to stay at the surface or close to it. Surface chemistry may thus modify transport phenomena what is a basically unexplored area. The proposed project ventures into this exploration focusing on metal alloys that are known in metallurgy as non-miscible. Various metals may offer specific mechanical, optical, magnetic, electric or catalytic properties, mixing them is often favorable so the inability to mix is a bad news. Luckily people have found various smart ways to mix them in nanocrystalline form and such products have found many applications. Heating such mixtures leads usually to a quick phase separation wrecking the desired properties.

All mentioned above diffusion phenomena at ambient temperatures run extremely slow. For nanocrystals however even diffusion path of few nanometers can affect the product properties. Research in this area including chemical factors influencing diffusion and phase separation may find ways to circumvent many such problems. The scope of the project encompasses determination of the diffusion kinetics of the component elements, growth kinetics, phase diagram exploration and deep insight into morphology of the evolving alloy. Surface characterization by measuring surface reactivity of the treated nanoalloy in some test reactions also is an important part of proposed studies.

Methodology: As we have already shown in a number of our publications a specially devised in situ X-ray powder diffraction technique (XRPD) combined with atomistic simulation tools is able to provide substantial insight into structural properties of nanoalloys. This methodology is continuously developed by us. The project assumes repeatable long time monitoring of slow diffusion processes following their kinetics and response to changing chemical environment. We will employ a dedicated diffractometer and constructed in our laboratory XRPD environmental chamber together with mass spectrometer and gas feeding system forming automatic, programmable system. Experiment oriented merger of measurement and theoretical methods used in our group provides innovative, attractive and potent methodology..

Expected impact on the development of science: A recent search for nanomaterials offering new, unknown in bulk form properties has to consider their long term durability. Slow diffusion phenomena may involve atom migration over distances comparable with the nanocrystal size. As the nanomaterial properties can depend on the grain boundaries (e.g. collecting impurities or affected by adsorption) such diffusion may ruin the devised properties. Understanding and prediction of such processes is thus fundamental. The experiments on small size nanoalloys may also provide diffusion characteristics not available otherwise but of importance for engineering of nanomaterials thus offering practical application.The results will expand knowledge of thermodynamics of small alloy systems.