METASTABLE EMBEDDED NANOPARTICLES IN METALLIC ALLOYS. GENERAL CONCEPTS AND ATOMISTIC MODELING.

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Nanoscale inhomogeneities are typical for numerous metallic alloys and crucially important for their practical applications [1]. This kind of structural state can be formed due to freezing/ stabilization of an incomplete stage of the phase transformation or due to formation long-living metastable nanosized-scale precipitates embedded in a host. This a heterogeneous state was observed in many technologically important alloys (Guinier-Preston zones in Al alloys, athermal omega-phase in Ti- and Zr-based alloys, precipitates of Co in Cu and other). However, the mechanism of formation and stabilization such state are still poorly understood.

Here we present an overview of the problem, together with a discussion of the typical examples of heterogeneous states. It is demonstrated, the stability of such precipitates is controlled by competition between short-range (chemical) and long-range (elastic) contributions to the free energy. We show that many–body interactions, including the contributions due to lattice relaxations, are mainly responsible for the formation of metastable planar (GPZ) atomic arrangements [2] and the kinetics of their formation can include several stages [3]. We discussed possible mechanisms of stabilization embedded nanoparticles and establish that it is controlled by removing long-range stresses due to loss of coherence [1] or/and segregation of alloying elements on the interface.

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1. Yu.N. Gornostyrev, M.I. Katsnelson, Phys. Chem. Chem. Phys., **17**, 27249 (2015)
2. O.I. Gorbatov, Yu.N. Gornostyrev, P.A. Korzhavyi, Scripta Materialia, **138**, 130 (2017)
3. A.Yu. Stroev, O.I. Gorbatov, Yu.N. Gornostyrev, P.A. Korzhavyi, Phys Rev Materials, **2**, 033603 (2018)