The Computational Materials Science Unit Colloquium

理論計算科学ユニットコロキウム

Date & Time: December 19th (Fri.) 3:00 pm – 4:00 pm

Place: Seminar room, Theoretical Research Building, Namiki site

Speaker: Prof. Alexander Umantsev, Fayetteville State University

Theory of Amorphous Nanophases

A number of very different recent experiments with nanoparticles (NPs) produced very similar results: in NPs of sizes above critical the sequence of transformations is similar to that of the bulk while in NPs of sizes below the critical a novel, *amorphous (disordered) phase* appears and remains stable in a significant domain of variation of the control parameters. A natural question arises: What is the origin of this phase? In a series of recent publications the author has developed a theory of the nanophase stability, which claims that the phase that appears in NPs of sizes below the critical is a *transition state* between the stable bulk phases in the space of the order parameter that distinguishes between the symmetries of the bulk phases. Such change of stability of the transition state from unstable to stable can occur only in conditions of conservation: energy [1, 4], matter [1, 2], or volume [1, 3]. As known, in large systems with the conservation constraint the transformation will result in a two-phase state, which is a mixture of the two stable bulk phases. The theory claims that in a system of the size below the critical such state is energetically impossible due to high 'energy cost' of the phase separating *interface*. Then, the two-phase state is replaced by the homogeneous transition state.

1. "Unusual Phases at Nanoscale", In *Dekker Encyclopedia of Nanoscience and Nanotechnology*, Ed. S. E. Lyshevski. In press (2014).
2. "Nanophases of Binary and Multicomponent Alloys". Acta Mater., **61**, 1106-1117 (2013). http://dx.doi.org/10.1016/j.actamat.2012.10.016
3. "Thermodynamic Stability of Transition States in Nanosystems", J. Stat. Phys., **136**, 117 (2009). http://www.springerlink.com/content/443u7h5658624803/
4. "Adiabatic phase transformations in confinement", J. Chem. Phys., **107**(5), 1600-1616, (1997). http://jcp.aip.org/resource/1/jcpsa6/v107/i5/p1600_s1

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