UDC 538.9

CLASSICAL NUCLEATION THEORY AND STOCHASTIC KINETIC MEAN FIELD APPROACH

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The nucleation stage of the first-order phase transformations in alloys is crucial for the prediction of mechanical, electrical, and magnetic properties of multiphase materials. During the last decades, new experimental possibilities have been developed enabling direct observation of nuclei formation during aging and solid-state reactions. Yet many details of the nucleation stage still remain a mystery.

The two most widespread methods of nucleation kinetics investigation are the Fokker – Plank approach and Monte Carlo simulation. The Fokker – Plank approach seems a good solution but it contains a number of not very well-determined parameters and not very well-proved phenomenological assumptions. Monte Carlo is more direct and atomistic, but the level of fluctuations in this method is so high that it is very difficult to distinguish the structures in small volumes.

Recently, our team along with the team of Debrecen University developed a new method called Stochastic Kinetic Mean Field (SKMF) [1 – 3]. This method combines George Martin`s mean field atomistic approach with the noise of local atomic fluxes. SKMF approach is inherently nonlinear and therefore applicable to the early stages of solid-state reactions under a sharp concentration gradient. Within this approach, the probability of atomic exchanges is proportional to the difference of exponents of chemical potentials, instead of the difference of just chemical potentials. Moreover, noise is introduced directly into atomic jumps quantity, instead of noise of composition.

Stochastic Kinetic Mean Field modeling on nucleation in supersaturated solution demonstrates the validity of Classical Nucleation Theory. The nucleation process consists of two main steps: at first, the embryo of the new phase appears with almost optimal composition and then this embryo increases its size at almost constant composition. The logarithm of nucleation time is inversely proportional to the squared supersaturation. The logarithm of nucleation time is a linear function of the inverse squared noise amplitude.

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3. *Bezpalchuk V., Abdank-Kozubski R., Pasichnyy M., Gusak A.* Tracer diffusion and ordering in fcc structures – stochastic kinetic mean-field method vs. kinetic monte carlo // Defect and Diffusion Forum. – 2018. – **383**. – P. 59–65.