The Computational Materials Science Unit Colloquium

理論計算科学ユニットコロキウム

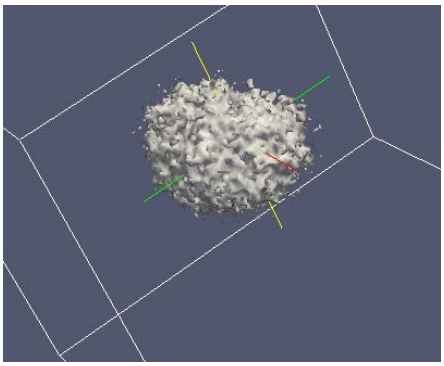
Date & Time: December 22nd (Mon.) 4:00 pm – 5:00 pm

Place: Seminar room, Theoretical Research Building, Namiki site

Speaker: Prof. Alexander Umantsev, Fayetteville State University

Modeling of Nucleation in Materials at Large Driving Forces

In many material systems the process of nucleation proceeds far away from equilibrium that is, at large driving forces, when the standard approach of the stationary nucleation rate is not applicable. Examples are crystallization of organic fluids, colloids, low dimensional systems, etc. In this project we develop an approach based on the concept of lifetime of a metastable state. We use the Ginzburg-Landau-Langevin method where the internal thermal noise is modeled as an additional stochastic force of specified intensity. To calibrate the method we calculate the equilibrium properties of the metastable state using the perturbation theory and Feynman diagrams and compare the results with the simulated ones. Then we use our method to calculate the lifetime of a metastable state as a function of the supersaturation, noise intensity, and system size. We analyze the 3D structure of the critical nuclei and find them to have large degree of ramification. Applications to materials problems will be discussed.



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