

Nucleation on surface with heterogeneous surface energy in Ising model

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First order phase transitions begin with a stage of nucleation, when individual particles form small domains of the new phase within the metastable old phase. Basics of this process can be described using the classical nucleation theory, but in some more complex nucleation scenarios, necessary modifications of theory were often hard to test experimentally. In such cases computer simulations can be very useful.

We utilize Ising model to study a specific case of nucleation scenario: nucleation in the presence of an inhomogeneous surface energy. The results are obtained using Monte Carlo simulation in lattice Ising model with spin-flip dynamics, utilizing the Umbrella sampling as a method to overcome difficulties with simulation of rare events. We also utilize corrected cluster-counting algorithm, leading to different results from so called "geometrical cluster" count.

Several cases of inhomogeneous surface energy were studied: array of regular bars of different energy, random noise, and a specific patterns designed in attempt to influence nucleation progress. Results mainly show that heterogeneity of the surface energy helps the nucleation process.

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