

## Formation Mechanism of Fe Nanocubes by Magnetron Sputtering Inert Gas Condensation

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Why do iron nanocubes form during condensation process instead of usual spherical or close-to-spherical shapes? It is counter-intuitive from the surface minimization considerations. We address this question by applying the combination of three different techniques: experiment, Molecular Dynamics and Kinetic Monte Carlo simulations. By these method we study kinetics of the formation mechanism of iron nanocubes. Our experiments as well as computer simulations indicate that the cubic shape of iron nanoparticles is explained by the difference in the kinetic growth modes of (100) and (110) surfaces, rather than the surface formation energetics. Our results are in good agreement between the different methods, showing that the final shape is defined by condensation temperature in combination with deposition rate. We present also the full deposition rate–temperature diagram of iron nanocluster shapes as well as an analytical model predicting the temperature and deposition rate evolution in nanoparticles. Combined together, the diagram and the model can be used to tune the desired final shape of the grown iron nanoparticles.

[1] J. Zhao, E. Baibuz, J. Vernieres, P. Grammatikopoulos, V. Jansson, M. Nagel, S. Steinhauer, M. Sowwan, A. Kuronen, K. Nordlund, and F. Djurabekova, *ACS Nano* **10**(4), 4684 (2016).