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"The Nucleation of Crystals: Simple Models for a Complex Problem"

Crystallisation is an important and widespread phenomenon. For example, most drugs are sold as crystals and so must be controllably crystallised, and models of the Earth's atmosphere require as input the rates of freezing of water droplets. The freezing of water droplets is an essential process in cold clouds. Crystallisation starts with an activated process: nucleation. I will mainly discuss statistical models of nucleation, particularly the role of quenched disorder, but I will also show the results of computer simulation of nucleation. Quenched disorder is disorder in the system that is fixed, i.e., it does not vary in time, as thermal fluctuations do.

Nucleation can be complex. Recent experimental results for both aspirin [1] and water [2] crystallisation, and simulation results on a lattice model with quenched disorder [3] are not consistent with a nucleation rate that is in the thermodynamic limit. This has consequences, if the rate is not in the thermodynamic limit, the time for nucleation will not necessarily scale as one over system size.

I will introduce the statistics required to analyse data for nucleation times to test for the existence of a well defined nucleation rate. I will introduce the use of extreme-value statistics to model the quenched disorder. I will introduce extreme-value statistics, which is useful in a number of of fields of physics, and use it to make predictions for nucleation that are testable in experiment.

I will also discuss the calculation of nucleation rates via computer simulations of simple models, and give some examples of a crystal nucleating on a surface that is also crystalline. Then the match between the crystal lattice of the nucleus and the lattice of the surface is important.

[1] Y. Diao,et al., J. Am. Chem. Soc. 133, 3756 (2011).
[2] S. L. Broadley et al., Atmos. Chem. Phys. 12, 287 (2012).
[3] R. P. Sear, J. Phys. Cond. Matt. 24 (2012) 052205
[4] R. P. Sear, Cryst. Growth Design 13, 1329 (2013).