Simulating nucleation in a driven system with Forward Flux Sampling: a two-dimensional Ising model under shear

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Rare events, which happen rapidly but infrequently, are notoriously difficult to simulate because few events are observed in a typical simulation run. This problem is particularly severe for driven systems, where the steady state phase space density is not known and rare event sampling methods such as the Bennett-Chandler method [6] and transition path sampling [7] cannot be used. We have recently developed a method, known as Forward Flux Sampling (FFS) [1, 2, 3], which can be applied to driven systems, since it does not require knowledge of the steady state phase space density.

In this work, we apply FFS to the problem of nucleation under shear in a two-dimensional Ising model. Most progress in understanding nucleation has been made for "quasi-equilibrium" systems, in which the system dynamics obeys detailed balance. Nucleation in driven systems is much less well understood, even though it is important for a wide range of industrial applications, as well as being of fundamental physical interest [5]. Our model system is highly simplified, but nevertheless shows rather complex behaviour.

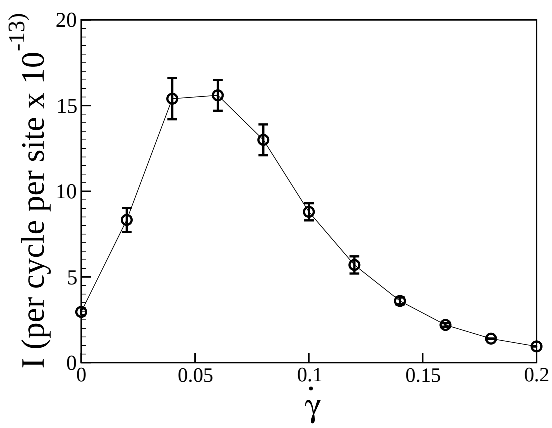

Figure 1: Nucleation rate I as a function of shear rate $\dot{\gamma}$.

We use a two-dimensional Ising model with Metropolis spin flip dynamics, $65 times 65$ spins, coupling parameter $\beta J = 0.65$ and external magnetic field $\beta h = 0.05$. We apply a linear velocity gradient to the system using a method similar to that of Cirillo et al. [4]. Figure 1 shows that the nucleation rate has a maximum value at intermediate shear rate. We show that this can be understood as a result of the interplay between shear-mediated cluster breakup at high shear, and shear-mediated cluster coalescence, as well as kink-mediated cluster growth, at low shear rates.

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REFERENCES

1. Allen, R. J, Warren, P. B., and ten Wolde, P. R. *Phys. Rev. Lett.*, **94**, 018104, (2005).
2. Allen, R. J, Frenkel, D, and ten Wolde, P. R. *J. Chem. Phys.*, **124**, 024102, (2006).
3. Allen, R. J, Frenkel, D, and ten Wolde, P. R. *J. Chem. Phys.*, **124**, 194111, (2006).
4. Cirillo, E. N. M, Gonella, G., and Saracco, G. P. *Phys. Rev. E*, **72**, 026139, (2005).
5. Onuki, A., *J. Phys. Condens. Matter*, **9**, 6119, (1997).
6. Frenkel, D., *Understanding Molecular Simulation*, Academic Press, Boston, (2002).
7. Dellago, C., Bolhuis, P. G., and Geissler, P. G. *Adv. Chem. Phys.*, **123**, 1, (2002).