

Molecular Dynamics Simulation of Spinodal Decomposition in a Two-Dimensional Binary Fluid Mixture

In the recent Letter [1], the authors report the existence of a novel “fast” scaling regime in a molecular dynamics (MD) simulation of a two-dimensional Lennard-Jones-like binary fluid mixture, in which the typical domain size R scales with time t as $R \sim t^\alpha$, with an exponent $\alpha = 0.65$. Reference [1] also reports a slower growth regime preceding the faster growth, characterized by an exponent $\alpha = 1/4$, as well as an early-time growth exponent $\alpha = 1/2$. They base these conclusions on individual runs using a variety of MD simulation techniques.

Here we argue that the scaling behavior they observed may be an artifact of their simulations. We find that although individual runs exhibit anomalous features of the sort found in [1], these features do not survive an averaging process over several independent realizations.

We have repeated the MD simulations of [1] using the velocity rescaling technique (the technique used for “Run B” in [1]) for 12 independent samples of 17 000 particles each. As in [1], we truncated the Lennard-Jones-like potentials between the different particle types at 4.2σ and quenched each system from a high temperature to a low temperature $k_B T/\epsilon = 2$ at a density $\rho\sigma^2 = 0.4$. We took one time step to be 0.01 in reduced units and performed 60 000 time steps for each sample. We ran our simulations on 16 nodes of a Connection Machine CM-5, using a MIMD algorithm implemented in CM Fortran, and consumed a total of 84 hours of CPU time. This algorithm achieves an update time of 25 μ s per particle.

Figure 1 shows the dependence on t of the typical domain size, R , as estimated by calculating the first zero of the pair correlation function $g(r)$ [2]. Shown are selected data from individual runs as well as the average over all 12 runs. The figure shows that individual runs differ significantly from one another. In fact, data set No. 3 resembles that of run B in Ref. [1]. However, when we average over all 12 data sets, there is no evidence of either a fast growth regime with exponent $\alpha = 0.65$ or a slow growth regime with $\alpha = 1/4$, reported in [1]. Instead, we find an exponent $\alpha = 0.49$ over the entire range of data, consistent with the “hydrodynamic” prediction [3] of $\alpha = 1/2$.

We thank E. Velasco and S. Toxvaerd for their generous cooperation in resolving this issue, the Center for Computational Science at Boston University for computational resources, and the National Science Foundation. Additionally, S.C.G. would like to thank J. F. Douglas

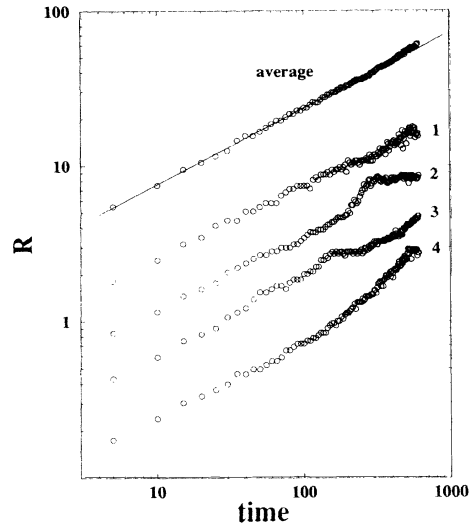


FIG. 1. Typical domain size, R , plotted log-log versus time t . The topmost line of data points represent an average over 12 independent samples, while the other points indicate individual runs. The vertical axis is shifted for each set of data to allow for direct comparison. The solid line is the best fit to the averaged data and has a slope 0.49.

and R. D. Mountain for useful discussions, and the NRC for Postdoctoral Fellow support.

Peter Ossadnik, Mark F. Gyure, and H. Eugene Stanley
Center for Polymer Studies
Boston University
Boston, Massachusetts 02215

Sharon C. Glotzer
National Institute of Standards and Technology
Polymers Division
Gaithersburg, Maryland 20899

Received 29 October 1993;
revised manuscript received 2 March 1994
PACS numbers: 61.46.+w, 31.20.Sy, 63.20.Kr, 74.70.Wz

- [1] E. Velasco and S. Toxvaerd, Phys. Rev. Lett. **71**, 388 (1993).
- [2] T. M. Rogers, K. R. Elder, and R. C. Desai, Phys. Rev. B **37**, 9638 (1988).
- [3] M. San Miguel, M. Grant, and J. D. Gunton, Phys. Rev. A **31**, 1001 (1985).