Computer Simulations, Nucleation Rate Predictions and Scaling

BARBARA   HALE, University of Missouri-Rolla — Computer simulations which
generate small molecular cluster size distributions for use in steady state nucleation
rate predictions and direct molecular dynamics simulations of the nucleation process
depend crucially on the properties of the effective pair potentials and on the mod-
eled system's metastable conditions. The latter conditions often differ significantly
from those under which the experimental data are taken. For argon, in particular,
simulations using both truncated and full Lennard-Jones potentials have generated
a range of results for the nucleation rate, J, which, in magnitude, appear to be in-
consistent with the limited experimental rate data. We propose that log J should
be plotted *versus* a "universal" function of the scaled supersaturation, $\ln S/[T_c/T - 1]^{3/2}$, which incorporates scaling of metastable system conditions with potential
model (or experimental) properties, as appropriate. This plot, which provides a more
realistic comparison of predicted and experimental rates, is applied to water and to
argon data. For argon, this plot emphasizes the limited range of simulation results
at large scaled supersaturations and suggests that none of these predicted rates are
inconsistent with the much smaller experimental nucleation rates taken at reduced
scaled supersaturations. For water, the plot indicates that experimental nucleation
rates are likewise well characterized by the scaled supersaturation function.

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