Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Combining Coarse-Graining and Density of States Monte Carlo: Application to Ortho-terphenyl JAYEETA GHOSH, ROLAND FALLER, UC Davis — The non equilibrium transition from liquid to glass is a challenging problem in condensed matter physics. Various techniques have been applied to elucidate the nature of transition without reaching consensus. The relevant time scales near the glass transition are so long that Molecular Dynamics fails. There is much debate whether standard Monte Carlo succeeds can sample phase space near or below the glass transition temperature. We therefore combine advanced techniques to study the system near the glass transition temperature. Based on atomistic models of the small organic glass former Ortho-terphenyl (OTP) we develop a mesoscale model in which each phenyl ring is replaced by a single interaction center. We obtain a structurally coarse-grained model based on Boltzmann inversion of atomistic radial distribution function at various temperatures. As atomistic radial distribution functions are only weakly temperature dependant, the optimization can be performed at any temperature and can be used for a range of temperatures. It turned out that in the glassy range we need to optimize the potential below the glass transition temperature. Once we have a valid mesoscale model we apply the Wang-Landau Density of States Monte Carlo technique to find the density of states for the system. This novel Monte Carlo technique has already been applied to model glass forming materials but not yet to a chemically explicit model.

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Date submitted: 08 Nov 2006 Electronic form version 1.4