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Correlations of System Mobility with Various Scalar Metrics
JULIEANNE HEFFERNAN, ROBERT BACA, JOHN MCCOY, New Mexico Institute of Mining and Technology, JOANNE BUDZIEN, DOUGLAS ADOLF, Sandia National Laboratories — Molecular dynamic simulations of chain systems were performed in order to investigate the relationships between the system mobility and thermostatic quantities. Systems consisted of pearl-necklace chains along with single site penetrants. Both attractive and repulsive systems (based on the cut-off of the Lennard-Jones potential) were simulated. The diffusion coefficients, D, for the chains and penetrants were then found for a variety of temperatures (T) and density combinations. D/T was found to be a single-valued function of a thermostatic quantity that we denoted as a "scalar metric." Four scalar metrics were found. Since, through the master curve, the mobilities for all temperature-density points can be extrapolated to a single zero, a unique ideal glass transition can be proposed to exist. Consequently, a scalar metric can be used as a "distance" measure to this ideal glass transition.

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