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Dynamics in a meta-basin and its relation to β relaxation in glass-forming liquids CHANDAN DASGUPTA, PRANABJYOTI BHUYAN, Indian Institute of Science, Bangalore, India — A clear interpretation of the short-time β relaxation of glass-forming liquids in terms of dynamics in the potential energy landscape is not yet available. We have studied the relation between dynamics in a meta-basin of the potential energy landscape and β relaxation in a well-known glass-forming liquid - the Kob-Andersen binary mixture. Meta-basins are determined from the series of inherent structures obtained by minimizing the potential energy, starting from configurations obtained from a constant-temperature molecular dynamics (MD) simulation. The eigenvalues and eigenvectors of the Hessian matrices of the inherent structures in a meta-basin are then used to calculate various dynamical quantities in the harmonic approximation. We find that the results of the harmonic calculation begin to deviate from those obtained from MD simulations at time scales substantially shorter than the β relaxation time corresponding to the plateau in the mean-square displacement versus time plot. The agreement between the results of our analysis of the dynamics in a meta-basin and those of MD simulations is found to extend to longer times when anharmonic effects are included in the analysis. A detailed comparison between these two set of results will be presented.

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