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Local activated dynamics in liquids TAKUYA IWASHITA, University of Tennessee, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — Transport properties of glass-forming liquids, such as viscosity and diffusion, are an important and unsolved subject in condensed matter physics, and in particular the quantitative description of the dynamics of such liquids still remains incomplete. We studied the local activation process in a liquid in terms of the change in local coordination number Nc, which is the number of nearest neighbor atoms. We calculated the transition rate between Nc coordinated state and (Nc+1) or (Nc-1) coordinated state in 3D molecular dynamics simulation. The transition rate is dependent on Nc, and as temperature is lowered the transition rate exhibits a strong dependence on Nc, indicating the system becomes more heterogeneous at the atomic level. The analysis allows us to determine local activation energy as a function of temperature and Nc, and in Nc-configuration space a local energy landscape picture was constructed as a new conceptual view of liquid dynamics. This result provides an interesting and fundamental framework for describing the dynamics of liquids. We also discuss the principle of detailed balance for the transition rate in liquids.

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