

Abstract Submitted
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Configurational excitations of simple liquids TAKUYA IWASHITA, University of Tennessee, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — The dynamics of glass-forming liquids has not been fully understood at the atomic-scale level, even for normal liquids because the basic mechanism regarding to liquid dynamics remain unknown. An elementary process of liquids, in which an atom loses or gains one of its nearest neighbors, was studied using MD simulations of various metallic liquids at high temperatures. The result was presented in terms of Maxwell relaxation time, represented by viscosity/G, and the lifetime of local topology of atomic connectivity. Above crossover temperature, T_A , the Maxwell relaxation time is almost equal to the lifetime of local topology, suggesting the topological excitation as the elementary excitation in high temperature liquid metal. We also showed that the T_A may be associated with the propagation of transverse sound wave beyond an atomic shell. Below T_A the Maxwell relaxation time becomes larger than the lifetime of local topology. This result implies an importance of the interaction between local configurational excitations in the supercooled state.

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