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Is microscopic description of inherent structures possible? VALENTIN A. LEVASHOV, TAKESHI EGAMI, Univ. of Tennessee, RACHEL S. AGA, JAMES R. MORRIS, Oak Ridge National Laboratory — Description of relaxation in a supercooled liquid of N particles using 3N dimensional potential energy landscape (PEL) implicitly favors the idea that the structure is too complex to be described by any microscopic local structural parameters. We addressed this issue by using atomic level stresses (ALS) introduced a while ago as local structural parameters. With MD simulations and the steepest decent method on a model of liquid iron we studied how the distributions of ALS in inherent structures (IS) depend on the original temperature. We found that the ALS of the IS clearly show the crossover and glass transition temperatures. Thus we conclude that relaxation in inherent structures could be described not only by macroscopic, but also by microscopic topological quantities (MTQ). We also found a way to relate the character of fluctuations in MTQ at real temperatures to the energies of the corresponding IS. We found that the mode-coupling temperature is located significantly below the crossover temperature, closer to the glass transition temperature.

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