

Energy Landscape Statistics and Coarsening in Liquids and Glasses – a Relaxation Mode Analysis

Yang Zhang^{1, 2}

¹ Department of Nuclear, Plasma, and Radiological Engineering and ²
Department of Materials Science and Engineering, University of Illinois at
Urbana-Champaign

Energy landscape, the hyper-dimensional manifold in the configurational space, has been a useful concept in describing complex processes that occur over a very long time scale, such as the multistep slow relaxations of supercooled liquids, folding of polypeptide chains into structured proteins, aging and degradation of materials, and mathematical optimizations. However, it remains a challenge how to quantify the energy landscape experimentally. In the last couple of years, we developed a relaxation mode analysis (RMA) method for liquids under a framework analogous to the normal mode analysis in solids. Using RMA, we show important statistics of the activation barriers of the energy landscape can be readily obtained from the experimentally measurable two-point correlation functions, e.g. using quasi-elastic and inelastic scattering experiments. We observed a prominent coarsening effect of the energy landscape. The results are further confirmed by direct sampling of the energy landscape using a metadynamics-like adaptive autonomous basic climbing computation. In this talk, I will first demonstrate this approach in the case of supercooled liquids when dynamical cooperativity emerges in the landscape-influenced regime. Then I will show, using this framework, we are able to extract the energy landscape statistics of a complicated confined protein system, which shows great promises for protein preservation.