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How deformation enhances mobility in a polymer glass

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Recent experiments show that deformation of a polymer glass can lead to orders-of-magnitude enhancement in the atomic level dynamics. To determine why this change in dynamics occurs, we carry out molecular dynamics simulations and energy landscape analyses. The simulations address the coarse-grained polystyrene model of Kremer and co-workers, and the dynamics, as quantified by the van Hove function, are examined as the glass undergoes shear deformation. In agreement with experiment, the simulations find that deformation enhances the atomic mobility. The enhanced mobility is shown to arise from two mechanisms: First, active deformation continually reduces barriers for hopping events, and the importance of this mechanism is modulated by the rate of thermally activated transitions between adjacent energy minima. Second, deformation moves the system to higher-energy regions of the energy landscape, characterized by lower barriers. Both mechanisms enhance the dynamics during deformation, and the second mechanism is also relevant after deformation has ceased.