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Energy Barriers for Defects in Disordered Solids SVEN WIJTMANS, LISA MANNING, Syracuse University — In solids, defects govern flow and failure. In crystals, defects are easily-identified dislocations, while in disordered solids, defects can be found by analyzing the vibrational modes of the system, which are eigenvectors of the matrix describing the linear response. The low frequency modes are typically quasi-localized hybrids of excitations localized at the defects and plane-wave like modes. Additional analysis can separate these components, giving the location of a defect and displacement of particles along that defect. To define an energy barrier for each defect, we displace particles along an isolated defect mode and calculate the energy at which the system transitions to a new energy basin. Different definitions of a new basin, such as a change in the particle contact network or particle displacements above a specific threshold, give different results. We identify several criteria that are consistent and provide a reasonable, robust definition of an energy barrier. Somewhat surprisingly, we find that energy barriers for isolated defects are generally higher than energy barriers for typical quasi-localized modes in the system.

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