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Strain-rate and temperature-driven transition in the shear transformation zone PENGHUI CAO, XI LIN, HAROLD S. PARK, Department of Mechanical Engineering, Boston University — We couple the recently developed self-learning metabasin escape algorithm, which enables efficient exploration of the potential energy surface (PES), with shear deformation to elucidate strain-rate and temperature effects on the shear transformation zone (STZ) characteristics in two-dimensional amorphous solids. In doing so, we report a transition in the STZ characteristics that can be obtained through either increasing the temperature or decreasing the strain rate. The transition separates regions having two distinct STZ characteristics. Specifically, at high temperatures and high strain rates, we show that the STZs have characteristics identical to those that emerge from purely strain-driven, athermal quasistatic atomistic calculations. At lower temperatures and experimentally relevant strain rates, we use the newly coupled PES + shear deformation method to show that the STZs have characteristics identical to those that emerge from a purely thermally activated state.

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