Abstract Submitted
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An energy landscape description of the mechanical response of model glassy materials[1] MINGLEI WANG, KAI ZHANG, MENG FAN, YANHUI LIU, JAN SCHROERS, Yale Univ., MARK SHATTUCK, The City College of the City University of New York, COREY O'HERN, Yale Univ., CENTER FOR RESEARCH ON INTERFACE STRUCTURES AND PHENOMENA TEAM — We perform molecular dynamics simulations of binary Lennard-Jones glasses to determine their mechanical response over a range of cooling rates spanning more than three orders of magnitude. To quantify the mechanical response, we measure the shear and bulk moduli using pure shear and compression deformation modes. To correlate the mechanical response to properties of the energy landscape, we also perform zero-temperature quasistatic pure shear simulations and measure the energy per particle as a function of strain. We show that glasses quenched at slower rates possess more brittle response since they exist in deeper energy minima with wider basins. In contrast, rapidly quenched glasses possess ductile response since they exist in shallow, narrow energy minima, which are easily overcome through applied shear.

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