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Local collapse of the atomic cage in a liquid flow
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The local structure of a model glass under steady shear was studied by molecular dynamics simulation for both high (T>Tg) and low (T<Tg) temperature ranges. The local structure was presented in terms of the anisotropic pair-density function (PDF). We found that the local structure was strained over a limited range of distances, and the length-scale of the strained region was dependent on the strain rate, extrapolating to zero at a critical strain rate. A strong correlation between the local collapse, represented by cutting of the atomic bond, and the structural strain in the PDF was found. At low temperatures local failure happens in a serrated manner, caused mechanically by shear. At high temperatures the local failure occurs more randomly, which is governed by thermal fluctuation. An anomalous behavior was observed as temperature approaches to Tg. The results suggest that except for the supercooled state above Tg local failure occurs by cutting of a single bond. Only in the supercooled state multiple bonds have to be cut for flow to occur. A possible relation to the dynamic heterogeneity is discussed.

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