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Scalar softness field correlates to molecular rearrangements for a thermal polymer glass ANTON SMESSAERT, JÖRG ROTTLER, The University of British Columbia — A fundamental challenge in the field of amorphous materials is to understand the structural causes for the spatial distribution of plastic events. Recent studies suggest that the low frequency vibrational modes encode information about structurally weak regions. Such "soft spots" were shown to strongly correlate to molecular rearrangements for an athermal amorphous solid in 2D [1]. Building on these ideas, we construct a scalar "softness field" from a weighted superposition of low frequency modes and we show that this field identifies regions in which particles undergo rearrangements. We test the predictive strength of the field computationally for a 3D polymer glass model in a quiescent state at several temperatures. Rearrangements are identified as particle hops using a previously introduced detection algorithm [2]. We find that hops are clustered in regions of large softness, and present a quantitative analysis of the correlation. The autocorrelation of the field shows that the soft regions are long lived compared to the timescales of the rearrangements. Furthermore, we find that particles hop preferentially along soft directions that are predicted by the softness field.

[1] M.L. Manning & A.J. Liu,PRL 107,108302(2011)
[2] A. Smessaert & J. Rottler,PRE 88, 022314(2013)

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