Rearrangement dynamics in colloidal particle packings identified through local structure and machine-learning[1] ZOEY S. DAVIDSON, TIM STILL, MATTHEW D. GRATALE, XIAOGUANG MA, SAMUEL S. SCHOEN-HOLZ, DANIEL M. SUSSMAN, A.J. LIU, A.G. YODH, University of Pennsylvania — We explore the connection between measures of local structure and particle rearrangements in soft thermal quasi-two-dimensional colloidal systems employing a machine learning approach. Local structure is characterized by two and three point structure functions that measure radial and angular distributions of particles, and rearrangements are identified by a measure of change in average colloidal particle position. By generating labeled training data, we can extract the features of these functions that contribute to the likelihood of a rearrangement. In particular, we use a machine-learning algorithm to construct a decision function in the form of a scalar field we call softness that with high accuracy labels regions of particles more likely to rearrange. Thus, we can predict dynamic rearrangements from the instantaneous local structure. The softness field remains a good predictor when we vary the packing fraction between training and test data sets. In glassy samples, the softness field can identify aging as particles become less likely to undergo cage rearrangements.

Zoey S. Davidson
University of Pennsylvania

Date submitted: 05 Nov 2015   Electronic form version 1.4