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Efficient determination of soft spots in amorphous solids using local structural information EKIN CUBUK, Harvard University, SAMUEL SCHOENHOLZ, University of Pennsylvania, BRAD MALONE, Harvard University, ANDREA LIU, University of Pennsylvania, EFTHIMIOS KAXIRAS, Harvard University — Structural defects such as dislocations are also flow defects that control plastic flow in crystalline solids. In disordered solids, it is more challenging to identify such local regions that are susceptible to rearrangement. We propose an extremely fast method for identifying soft spots with high accuracy, which scales linearly with number of particles. We achieve this by training a supervised learning model with instances of local neighborhoods and their subsequent plastic flow behavior. By characterizing local neighborhoods with not just one structural quantity, such as bond orientational order, but a combination of multiple structural quantities, we are able to identify a population of regions that correlates just as strongly with rearrangements as do soft spots calculated from vibrational modes. This method does not require knowledge of the interparticle interactions and can readily be applied to experiments that measure the positions of constituent particles in a disordered packing. Furthermore, this also allows for the prediction of plastic behavior in systems like lithiated amorphous silicon, which is important for addressing the durability issues encountered in recent work on improving lithium-ion batteries.

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