Researchers establish universal signature fundamental to how glassy materials fail

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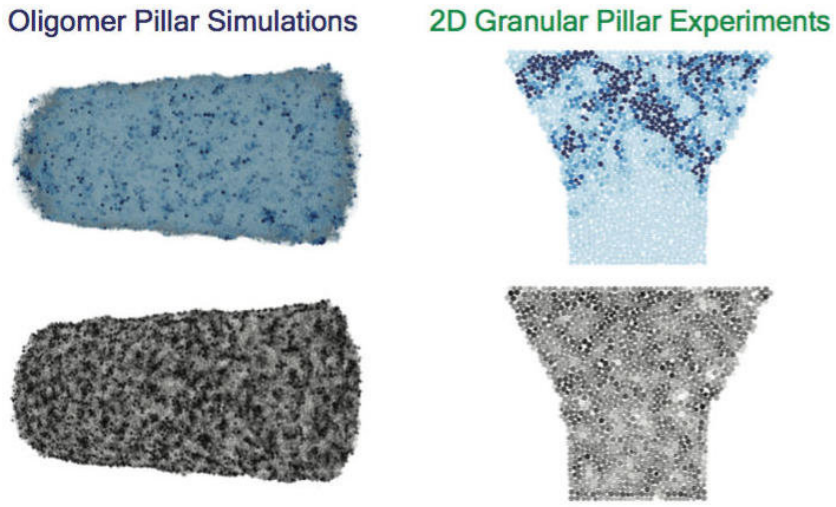


Snapshots of softness fields and particle arrangements for the oligomer pillar simulation and the granular pillar experiment, two of the systems investigated in the paper. Credit: University of Pennsylvania

Dropping a smartphone on its glass screen, which is made of atoms jammed together with no discernible order, could result in it shattering. Unlike metals and other crystalline material, glass and many other disordered solids cannot be deformed significantly before failing and, because of their lack of crystalline order, it is difficult to predict which

atoms would change during failure.

"In order to understand how a system chooses its rearrangement scenario," said Douglas Durian, professor of physics and astronomy at the University of Pennsylvania, "we must make connection with the underlying microscopic structure. For crystals, it's easy; rearrangements are at topological defects such as dislocations. For disordered solids, it's a very hard 40-year-old problem that we're now cracking: What and where are structural defects in something that's disordered?"

To find a link between seemingly disparate disordered materials, an interdisciplinary collaboration between Penn researchers in the School of Arts and Sciences and the School of Engineering and Applied Science with expertise in various materials studied an unprecedented range of disordered solids with constituent particles ranging from individual atoms to river rocks. Understanding materials failure on a fundamental level could pave the way for designing more shatter-resistant glasses or predicting geological phenomena like landslides.

In a paper published in *Science*, the Penn researchers revealed commonalities among these disordered systems, defining a counterpart to the "defects" implicated in crystalline materials failure. This so-called "softness" in disordered systems predicts the location of defects, which are the collection of particles most likely to change when the material fails.

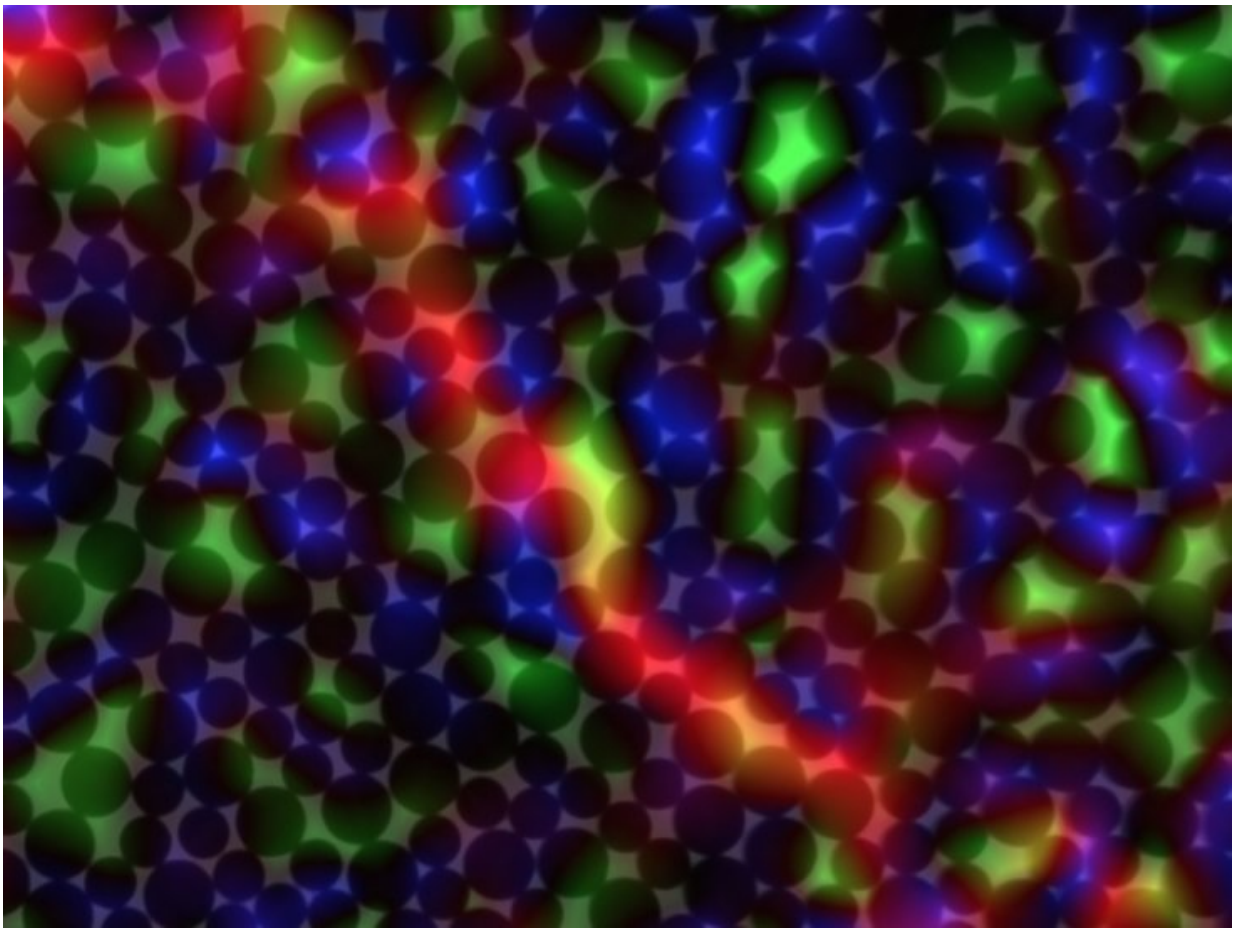
The researchers used a technique developed by Durian with Penn Ph.D. graduate Samuel Schoenholz, and Harvard University Ph.D. graduate Ekin Dogus Cubuk, both currently at Google Brain; Andrea Liu, Hepburn Professor of Physics in Penn's School of Arts and Sciences; and Efthimios Kaxiras, John Hasbrouck Van Vleck Professor of Pure and Applied Physics, Harvard School of Engineering and Applied Sciences. Liu and Daniel Gianola, then a professor in Penn's School of

Engineering and Applied Science's Department of Materials Science and Engineering and now at the University of California, Santa Barbara, led the study. Daniel Strickland and Robert Ivancic, both graduate students at Penn, are first authors, together with Cubuk and Schoenholz.

The paper is the culmination of years of research conducted at Penn's Materials Research Science & Engineering Center (MRSEC) which is hosted by the Laboratory for Research on the Structure of Matter. Liu and Robert Carpick, John Henry Towne Professor and chair in Mechanical Engineering and Applied Mechanics at Penn were co-leaders of the MRSEC's integrated research group focused on the mechanics of disordered packings.

A dozen of the group's faculty members, along with students and postdoctoral researchers from their labs, contributed to the study, providing data from 15 simulations and experiments on different types of disordered systems. The particles in those systems ranged in size from carbon atoms that make up wear-resistant engine coatings to centimeter-sized plastic spheres in a model riverbed.

Using machine learning, the researchers collected hundreds of quantities that characterize the arrangements of particles in each system, quantities that individually might not be expected to reveal much. Importantly, they found the combination of these quantities that correlates strongly with the dynamics. This produced a microscopic structural property called softness. If softness is known, the behavior of the disordered material and how likely its constituent particles are to rearrange can be predicted.



An image of the 2d granular system featured in the study. Blue shows overpacked regions, green shows under packed regions and red shows a transient shear band of the type the researchers are trying to understand. Credit: University of Pennsylvania

The systems the researchers studied were rearranging due to random thermal fluctuations or to different kinds of applied stress such as squeezing or stretching. In all cases, the technique worked well, and the researchers were able to predict with high accuracy the probability that the systems would rearrange.

The researchers then compared properties across systems. They found

that the length scale over which softness was correlated was identical to the size of rearrangements, or the number of particles that move when failure occurs. Remarkably, they found that this number is almost identical in all of these systems regardless of the size of the particles and how they interact.

"People have been talking about what sets the size of localized rearrangements in disordered solids for 40 years," Liu said. "They speculated about localized defects that they called shear transformation zones in disordered systems where rearrangements are likely to occur, but no one had seen this directly. They couldn't predict ahead of time where rearrangements would be likely to occur. With the machine learning, we're saying, 'Let's train the system. Let's look at the rearrangements and the structures and see if we can figure out what's important and then use that.' It's conceptually very straightforward, but it turns out to be very powerful."

The researchers also measured the yield strain, or how much the solid can be deformed before it starts to plastically deform. They also found that the yield strain is approximately the same for all disordered solids over systems spanning 13 orders of magnitude in their mechanical stiffness. By comparison, the yield strains for different crystalline materials can vary by a hundred- or thousand-fold.

Now that the researchers have shown that, up to and around when stress is applied, all these systems look the same, the next step of the effort is co-led by Durian and Paulo Arratia, professor of mechanical engineering and applied mechanics in the School of Engineering and Applied Science. Their goal is to go beyond yield, where all becomes chaos and the systems begin to look extremely different. Some systems fracture, others show shear bands and others, like foams, can smoothly flow forever.

"When a rearrangement happens, the softnesses of the nearby particles all change," Durian said, "but, due to long-range elastic couplings, so can the softnesses of particles even quite far away, as illustrated by this data. Thus, a rearrangement has a nontrivial effect on where the next rearrangements are likely to occur. In particular, will nearby rearrangements be encouraged and hence promote shear banding, or will they be discouraged and hence promote toughness? We believe that understanding and ultimately controlling the complex interplay between rearrangements, stress, and structure - here quantified by softness - is the key to improving toughness."

If the researchers can understand why different systems behave differently beyond yield, they may be able to control softness and how it evolves when it's under stress. This could lead to tougher coatings and materials, such as more durable glass screens for phones.

"Disordered solids have a lot of great properties," Liu said. "You can mold them into any shape you want or create surfaces that are atomically smooth, which you can't really do with crystalline systems. But they tend to shatter easily. If we can understand what controls that and how to prevent it, then the concepts start to have real applications. In an ideal case, we want to develop new, tougher materials that aren't as brittle or don't fall apart as catastrophically."

More information: E. D. Cubuk et al, Structure-property relationships from universal signatures of plasticity in disordered solids, *Science* (2017). DOI: 10.1126/science.aai8830

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