

Use machine learning to link atomic structure with glass properties and behaviors

Bu Wang, Dane Moran, Izabela Szlufarska, University of Wisconsin-Madison

Glasses have disordered arrangements of atoms without the repeating patterns that crystals have. However, there are small-scale patterns of atoms that touch each other which strongly affect the energy of the glass, how the atoms move when they get hot, and other properties like strength and response to an electric field. Unfortunately, there are many possible patterns and many slight variations of each one, so studying them is like sorting the grains of sand on a beach by size and color by hand—it's an impossible task.

Wisconsin MRSEC IRG 1 uses machine learning to sort the sand. They have developed algorithms to find small-scale atomic patterns in large simulations of glasses and link them to the glass' energy. Ongoing studies have connected patterns to atomic motions, which provides a path to simulations of glasses over long times and low temperatures that are currently impossible.

