UCLA Department of Physics & Astronomy

COLLOQUIUM

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Solving A Century-Old Problem: Three-Dimensional Atomic Structure of Amorphous Solids

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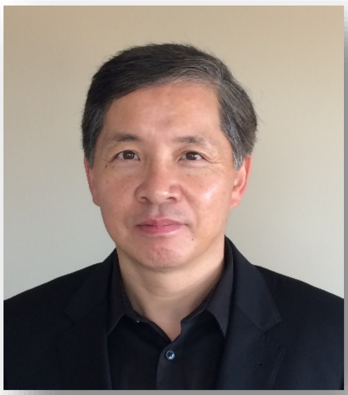

Liquids and solids are two fundamental states of matter. Although the structure of crystalline solids has long been solved, amorphous solids such as glass, rubber and plastics are more ubiquitous in our daily life and have broad applications ranging from telecommunications to electronics and solar cells. However, due to the lack of long-range order, the 3D atomic structure of amorphous solid had defied direct experimental determination for more than a century. As a graduate student, I aspired to solve this grand challenge in the physical sciences. In 1999, I pioneered coherent diffractive imaging (CDI) to extend X-ray crystallography to allow imaging of non-crystalline systems. In 2012, I applied CDI methods to tomography and pioneered atomic electron tomography (AET) to resolve the 3D atomic structure of matter without assuming crystallinity. In 2021, after more than 22 years of relentless pursuit, we finally advanced AET to determine the 3D atomic structure of a metallic glass and quantitatively characterized the short- and medium-range order. We discovered that, although the 3D atomic packing of the short-range order is geometrically disordered, some short-range-order structures connect with each other to form crystal-like superclusters and give rise to medium-range order. We identified four types of crystal-like medium-range order – face-centred cubic, hexagonal close-packed, body-centred cubic and simple cubic – coexisting in the amorphous sample, showing translational but not orientational order. These observations provide direct experimental evidence to support the general framework of the efficient cluster packing model for metallic glasses. Furthermore, we also used AET to resolve the 3D atomic packing in monatomic amorphous solids. We observed that pentagonal bipyramids are the most abundant atomic motifs in these amorphous solids. Instead of forming icosahedra, the majority of pentagonal bipyramids arrange into pentagonal bipyramid networks with medium-range order. Molecular dynamics simulations further reveal that pentagonal bipyramid networks are prevalent in monatomic metallic liquids, which rapidly grow in size and form more icosahedra during the quench from the liquid to the glass state. We expect that these results pave the way for the determination of the 3D atomic structure of a wide range of amorphous solids, which could transform our fundamental understanding of non-crystalline materials and related phenomena.

Undergraduates Welcome!