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Three-Dimensional Atomic Structure of Crystal Defects and Amorphous Materials

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Perfect crystals are rare in nature. Real materials often contain crystal defects, surface reconstructions, nanoscale heterogeneities and disorders, which strongly affect material properties and functionality. Although aberration-corrected TEM and STEM have been widely used to characterize materials at sub-angstrom resolution, they provide 2D projections of the materials. An approach to overcome this major limitation is atomic electron tomography (AET), which enables 3D structure determination of crystal defects and amorphous materials at atomic resolution. Over the last ten years, AET has been applied to image grain boundaries, anti-phase boundaries, stacking faults, dislocations, point defects, chemical order/disorder, atomic-scale ripples, bond distortion and strain tensors with unprecedented 3D detail. In this talk, I will report the 3D atomic positions of medium- and high-entropy alloys (M/HEA) nanocrystals determined by AET. We quantitatively characterize the local lattice distortion, strain tensor, twin boundaries, dislocation cores, and chemical short-range order (CSRO). We find that the local lattice distortion and strain tensor in the HEAs are larger and more heterogeneous than in the MEAs. We observe CSRO-mediated twinning in the MEAs, that is, twinning occurs in energetically unfavoured CSRO regions but not in energetically favoured CSRO ones. This observation confirms the atomistic simulation results of the MEA and represents the first experimental evidence of correlating local chemical order with structural defects in any material system. I will then present the 3D structure determination of metallic glass at atomic resolution and the quantitative characterization of 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. We expect that these results will pave the way for the determination of 3D atomic structures of a wide range of crystal defects and amorphous materials, which could transform our fundamental understanding of the structure-function relationships in materials science, chemistry, condensed matter physics, and nanoscience.

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