Atomic Scale Structural Characterization of Material Surfaces and Interfaces via Atomic Electron Tomography

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A high degree of anisotropy and even completely new phenomena can be often found at the materials surface/interface systems, and their properties are governed by the 3D arrangement of individual atoms at the surface/interface. To achieve a proper understanding of structure-property relations at the interface, a precise determination of the 3D interface atomic structures and their dynamics is a definite prerequisite, which has been limited to lower-dimensional measurements or simulations. Traditional crystallography, which is reliant on periodicity, cannot determine their real structures because the periodic symmetry breaks down at the surface/interface. Without any prior assumption of underlying structure, atomic electron tomography (AET) is now able to locate the 3D coordinates of individual atoms and their dynamics with picometer precision and with elemental specificity. A variety of complex internal atomic structures can be measured with 3D atomic-level details; including grain boundaries, chemical order/disorder and phase boundaries [1]. Recently, combined with deep-learning based neural network, it now became possible to precisely measure the 3D surface/interface structure of nanomaterials with high precision, revealing surface-substrate boundary effect, coalescence dynamics, core-shell strain relation and surface catalytic activity at the atomic scale [2-4]. Understanding the atomic resolution structural properties and their dynamics at the nanomaterial interfaces together with the relationship between atomic structure and material properties will allow the rational design of novel materials with desired surface/interface properties at the atomic scale.

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