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3D Structural Determination of Core-shell Nanoparticles

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By creating epitaxy between two different materials, the misfit strain at the interface can be finely controlled [1,2]. Core-shell architectures are prominent examples of such strain-engineered materials, where material properties can be designed by fine-tuning the misfit strain at the interface [3]. To fully utilize the interfacial strain effect, it is essential to have an atomic-scale understanding of their 3D interface structures. Here, we elucidate the full 3D atomic structure of Pd@Pt core-shell nanoparticles at the single-atom level via atomic electron tomography [4]. Full 3D displacement and strain maps of core-shell nanoparticles are obtained, which revealed a direct correlation between the surface and interface strains. It also shows clear Poisson effects at the scale of the full nanoparticle as well as the local atomic bonds. The strain distributions show a strong shape-dependent anisotropy, which is further corroborated by molecular statics simulations. From the observed surface strains, the surface oxygen reduction reaction activities were predicted [5]. These findings can give a deep understanding of structure-property relationships in core-shell systems, and suggest that the strain, as well as catalytic properties at the surface, can indeed be finely controlled through proper core-shell engineering.

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