3D atomic structure analysis of heterogeneous catalyst by “one-particle reconstruction”

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3D structures of heterogeneous catalyst typically deviate from the lattice structures measured and expected in their bulk counterparts. This is presumably because of the dominance of surface dangling bonds, defects, and dislocations within the volume of heterogeneous catalyst. To understand these unique structural features of heterogeneous catalyst, a method that can precisely determine the positions of the individual atoms is required. We introduce our experimental efforts using a combination of new techniques including graphene liquid cell for in situ TEM, aberration-corrected TEM, structure analysis algorithm, and 3D strain measurement. We apply it to determine the 3D atomic arrangements of different types of heterogeneous catalyst in solution. Our high-resolution 3D density maps and fitted atomic models show crystal structures of individual catalyst particles with structural degeneracies, including single crystalline, polycrystalline, distorted structures, and a dislocation. We also discuss the extent of this new analytical method regarding types and dimensions of materials systems which require unprecedented structural information in native conditions.