Observing individual atoms in 3D nanomaterials and their surfaces

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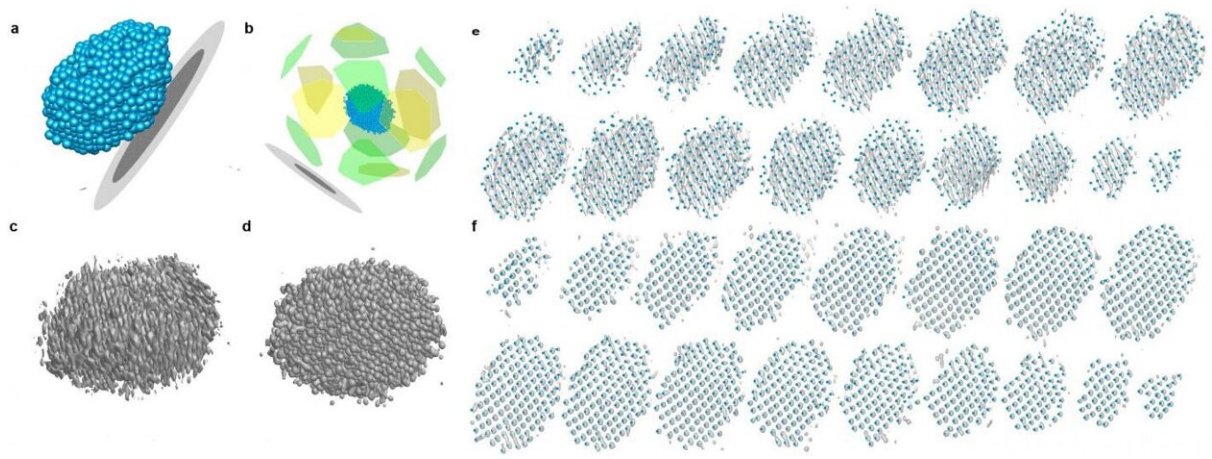

a. Overall atomic structure of a Pt nanoparticle determined in this study, with SiN substrate represented as black and gray disks. b. Identified facet structure of the Pt nanoparticle, showing all facets. c, d. Iso-surfaces of reconstructed 3D density from the electron tomography, before (c) and after (d) the deep-learning based augmentation, respectively. e, f. Tomographic reconstruction volume intensity and traced atom positions. Each slice represents an atomic layer, and the blue dots indicate the traced 3D atomic positions before (e) and after (f) the deep-learning based augmentation. The grayscale backgrounds are iso-surfaces of 3D density. Credit: KAIST

Atoms are the basic building blocks for all materials. To tailor functional properties, it is essential to accurately determine their atomic structures. KAIST researchers observed the 3D atomic structure of a nanoparticle at

the atom level via neural network-assisted atomic electron tomography.

Using a platinum nanoparticle as a model system, a research team led by Professor Yongsoo Yang demonstrated that an atomicity-based deep learning approach can reliably identify the 3D surface atomic structure with a precision of 15 picometers (only about 1/3 of a hydrogen atom's radius). The atomic displacement, strain, and facet analysis revealed that the surface atomic structure and strain are related to both the shape of the nanoparticle and the particle-substrate interface. This research was reported in *Nature Communications*.

Combined with quantum mechanical calculations such as density functional theory, the ability to precisely identify surface atomic structure will serve as a powerful key for understanding catalytic performance and oxidation effect.

"We solved the problem of determining the 3D surface atomic structure of nanomaterials in a reliable manner. It has been difficult to accurately measure the surface atomic structures due to the 'missing wedge problem' in electron tomography, which arises from geometrical limitations, allowing only part of a full tomographic angular range to be measured. We resolved the problem using a deep learning-based approach," explained Professor Yang.

The missing wedge problem results in elongation and ringing artifacts, negatively affecting the accuracy of the atomic structure determined from the tomogram, especially for identifying the surface structures. The missing wedge problem has been the main roadblock for the precise determination of the 3D surface atomic structures of nanomaterials.

The team used atomic electron tomography (AET), which is basically a very high-resolution CT scan for nanomaterials using transmission electron microscopes. AET allows individual atom level 3D atomic

structural determination.

"The main idea behind this deep learning-based approach is atomicity—the fact that all matter is composed of atoms. This means that true atomic resolution electron tomogram should only contain sharp 3D atomic potentials convolved with the electron beam profile," said Professor Yang.

"A deep neural network can be trained using simulated tomograms that suffer from missing wedges as inputs, and the ground truth 3D atomic volumes as targets. The trained deep learning network effectively augments the imperfect tomograms and removes the artifacts resulting from the missing wedge problem."

The precision of 3D atomic structure can be enhanced by nearly 70% by applying the deep learning-based augmentation. The accuracy of surface atom identification was also significantly improved.

Structure-property relationships of functional nanomaterials, especially the ones that strongly depend on the surface structures, such as catalytic properties for fuel-cell applications, can now be revealed at one of the most fundamental scales: the atomic scale.

Professor Yang concluded, "We would like to fully map out the 3D atomic structure with higher precision and better elemental specificity. And not being limited to atomic structures, we aim to measure the physical, chemical, and functional properties of nanomaterials at the 3D atomic scale by further advancing electron tomography techniques."

More information: Juhyeok Lee et al, Single-atom level determination of 3-dimensional surface atomic structure via neural network-assisted atomic electron tomography, *Nature Communications* (2021). DOI: 10.1038/s41467-021-22204-1