



For the first time scientists succeeded in determining the exact spatial arrangement of a single atom in a nanoparticle. The yellow spheres are the graphically depicted atoms that form the silver nanoparticle, which is about two nanometres in diameter. (Image: Empa/ETH Zürich)

# In atomic resolution

For the first time, scientists from Empa and ETH Zurich have, in collaboration with a Dutch team, managed to measure the atomic structure of individual nanoparticles. The technique, recently published in "Nature", could help better understand the properties of nanoparticles in future.

TEXT: Simone Ulmer\*

In chemical terms, nanoparticles have different properties from their "big brothers and sisters": they have a large surface area in relation to their tiny mass and at the same time a small number of atoms. This can produce quantum effects that lead to altered material properties. Ceramics made of nanomaterials can suddenly become bendy, for instance, or a gold nugget is gold-coloured while a nanosilver of it is reddish.

## New method developed

The chemical and physical properties of nanoparticles are determined by their exact three-dimensional morphology, atomic structure and especially their surface composition. In a study initiated by Rolf Erni, head of Empa's Electron Microscopy Center, and ETH Zurich scientist Marta Rossell the 3D structure of individual nanoparticles has now successfully been determined on the atomic level. The new technique could help improve our understanding of the characteristics of nanoparticles, including their reactivity and toxicity.

## Gentle imaging processing

For their electron-microscopic study, which was published recently in the journal "Nature", Rossell and Erni prepared silver nanoparticles in an aluminium matrix. The matrix makes it easier to tilt the nanoparticles under the electron beam in different crystallographic orientations whilst protecting the particles from damage by the electron beam. The basic prerequisite for the study was a special electron microscope that reaches a maximum resolution of less than 50 picometres. By way of comparison: the diameter of an atom measures about one Ångström, i.e. 100 picometres.

To protect the sample further, the electron microscope was set up in such a way as to also yield images at an atomic resolution with a lower accelerating voltage, namely 80 kilovolts. Normally, this kind of microscope – of which there are only a few in the world – works at 200 – 300 kilovolts. The two scientists used a microscope at the Lawrence Berkeley National Laboratory in California for their experiments. The experimental data was complemented with additional electron-microscopic measurements carried out at Empa.

## Sharper images

On the basis of these microscopic images, Sandra Van Aert from the University of Antwerp created models that "sharpened" the images and enabled them to be quantified: the refined images made it possible to count the individual silver atoms along different crystallographic directions.

For the three-dimensional reconstruction of the atomic arrangement in the nanoparticle, Rossell and Erni eventually enlisted the help of the tomography specialist Joost Batenburg from Amsterdam, who used the data to tomographically reconstruct the atomic structure of the nanoparticle based on a special mathematical algorithm. Only two images were sufficient to reconstruct the nanoparticle, which consists of 784 atoms. "Up until now, only the rough outlines of nanoparticles could be illustrated using many images from different perspectives", says Marta Rossell. Atomic structures, on the other hand, could only be simulated on the computer without an experimental basis.

"Applications for the method, such as characterising doped nanoparticles, are now on the cards", says Rolf Erni. For instance, the method could one day be used to determine which atom configurations become active on the surface of the nanoparticles if they have a toxic or catalytic effect. Rossell stresses that in principle the study can be applied to any type of nanoparticle. The prerequisite, however, is experimental data like that obtained in the study. //

## Literature reference

"Three-dimensional atomic imaging of crystalline nanoparticles", S. Van Aert, K.J. Batenburg, M.D. Rossell, R. Erni & G. Van Tendeloo, Nature (2011), doi:10.1038/nature09741

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