Researchers make first observation of atoms moving inside bulk material

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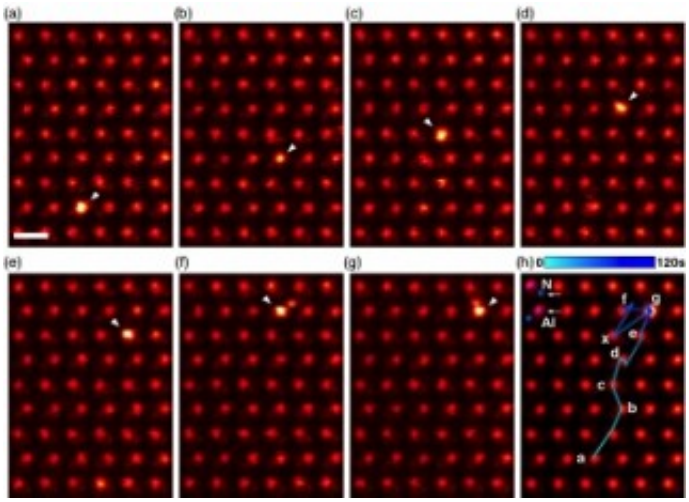

Selected frames from a sequence of scanning transmission electron microscope images showing the diffusion pathway of a Ce dopant (the bright atom highlighted with a white arrow) as it moves inside a bulk AlN crystal. The final frame overlays the Ce pathway on the Z-contrast image obtained by averaging each frame. Credit: Oak Ridge National Laboratory

Researchers at the Department of Energy's Oak Ridge National Laboratory have obtained the first direct observations of atomic diffusion inside a bulk material. The research, which could be used to give unprecedented insight into the lifespan and properties of new materials, is published in the journal *Physical Review Letters*.

"This is the first time that anyone has directly imaged single dopant

atoms moving around inside a material," said Rohan Mishra of Vanderbilt University who is also a visiting scientist in ORNL's Materials Science and Technology Division.

Semiconductors, which form the basis of modern electronics, are "doped" by adding a small number of impure atoms to tune their properties for specific applications. The study of the dopant atoms and how they move or "diffuse" inside a host lattice is a fundamental issue in materials research.

Traditionally, diffusion of atoms has been studied through indirect macroscopic methods or through theoretical calculations. Diffusion of single atoms has previously been directly observed only on the surface of materials.

The experiment also allowed the researchers to test a surprising prediction: Theory-based calculations for dopant motion in aluminum nitride predicted faster diffusion for cerium atoms than for manganese atoms. This prediction is surprising as cerium atoms are larger than manganese atoms.

"It's completely counterintuitive that a bigger, heavier atom would move faster than a smaller, lighter atom," said the Material Science and Technology Division's Andrew Lupini, a coauthor of the paper.

In the study, the researchers used a scanning transmission electron microscope to observe the diffusion processes of cerium and manganese dopant atoms. The images they captured showed that the larger cerium atoms readily diffused through the material, while the smaller manganese atoms remained fixed in place.

The team's work could be directly applied in basic material design and technologies such as energy-saving LED lights where dopants can affect

color and atom movement can determine the failure modes.

"Diffusion governs how dopants get inside a material and how they move," said Lupini. "Our study gives a strategy for choosing which dopants will lead to a longer device lifetime."

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