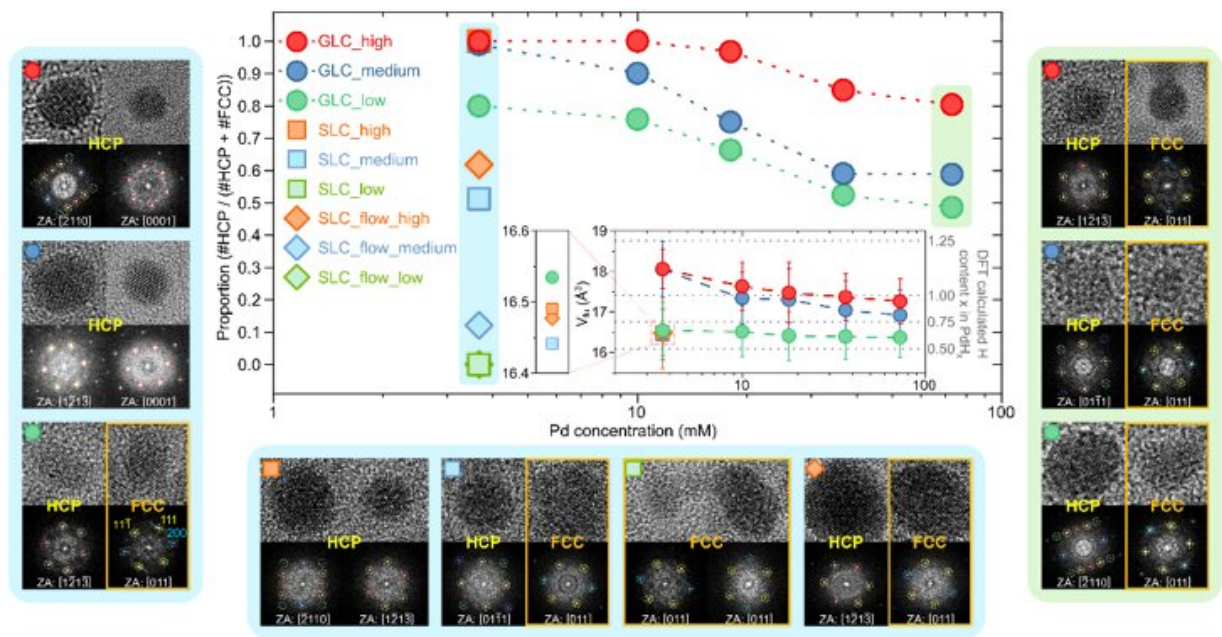


Development of metastable-phase advanced material synthesis technology

April 15 2022



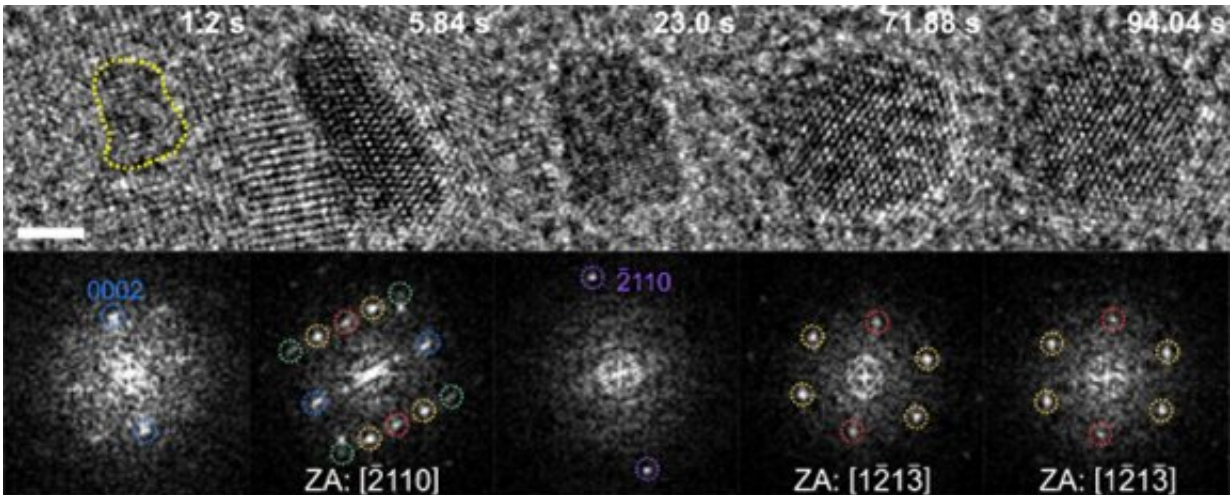
The percentage of metastable-phase palladium hydrides (HCP) generated depended on the palladium concentration in the palladium aqueous solution and the electron beam intensity and content of hydrogen within the metastable phase. The percentage of metastable-phase palladium hydrides (HCP) generated depended on the palladium concentration in the palladium aqueous solution and the electron beam intensity and content of hydrogen within the metastable phase. Credit: Korea Institute of Science and Technology

Similar to the widespread interest in graphite and diamond, there is

growing interest in metastable phases, which have different physical properties than those of stable phases. However, processes to fabricate metastable-phase materials are highly limited. New findings have been published in the latest issue of *Nature* about the development of a new metastable-phase synthesis method, which can drastically improve the physical properties of various materials.

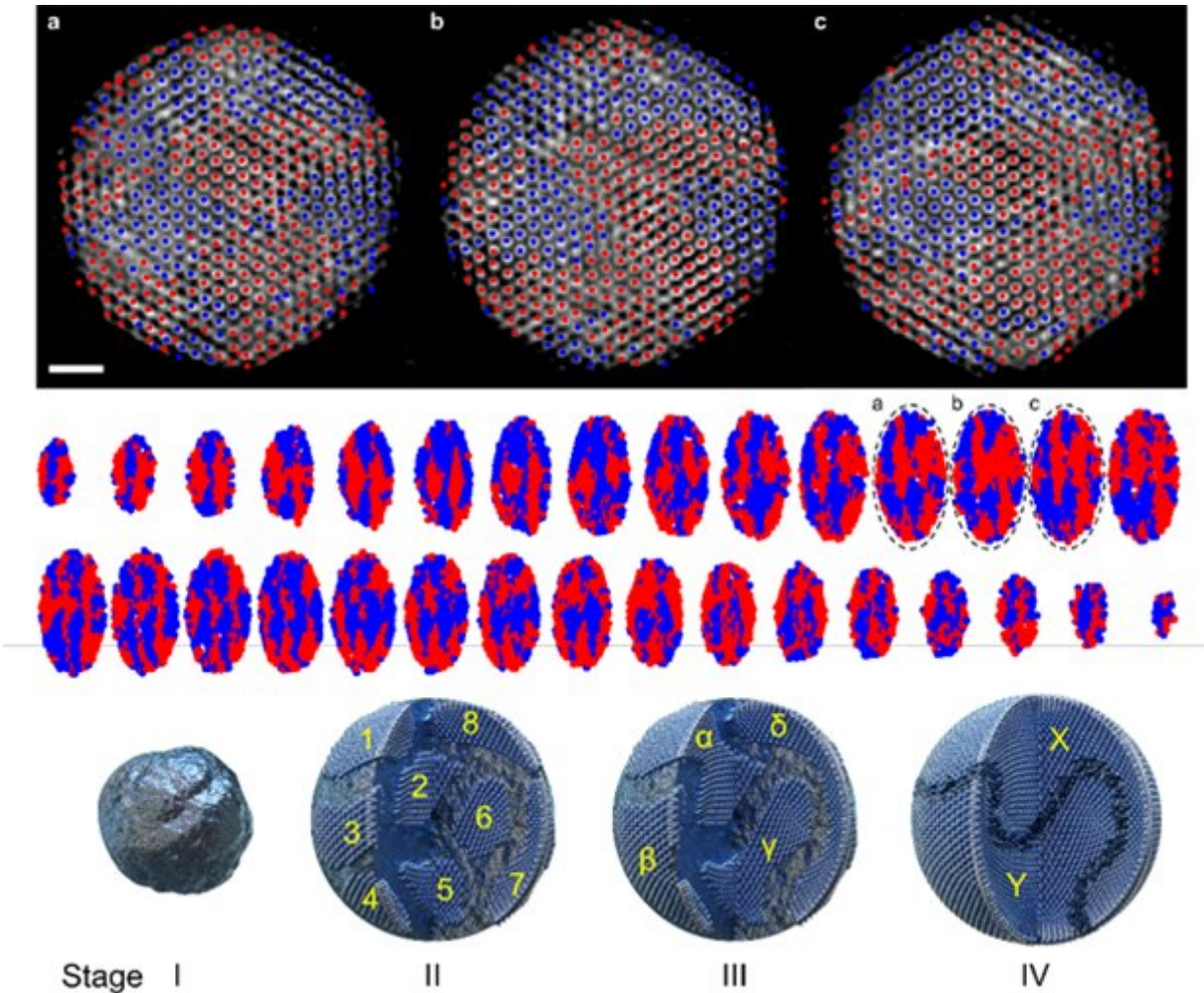
A research team led by Dr. Chun, Dong Won at the Clean Energy Research Division, Korea Institute of Science and Technology (KIST; President: Yoon, Seok Jin), announced that they successfully developed a new advanced metastable-phase palladium hydride (PdH_x) material. Furthermore, they identified its [growth mechanism](#).

A metastable-phase material has more thermodynamic [energy](#) than that in the stable phase but requires substantial energy to attain the stable phase, unlike most other materials, which exist in the stable phase with low thermodynamic energy. The research team directly synthesized a metal hydride by growing a material that can store [hydrogen](#) under a suitable hydrogen atmosphere, without dispersing hydrogen within a metal. Notably, they successfully developed a metastable-phase metal hydride with a new crystal structure. Further, they confirmed that the developed metastable-phase material had good thermal stability and twice the hydrogen storage capacity of a stable-phase material.



Real-time analysis of the growth process of metastable palladium hydride nanoparticles within a liquid phase by transmission electron microscopy. Credit: Korea Institute of Science and Technology

To elucidate the theoretical basis and scientific evidence for these findings, the research team used atomic electron tomography, which reconstitutes 3D images from 2D electron microscope images for nanometer-sized crystals in a metal hydrate, for analysis. As a result, they demonstrated that the metastable phase was thermodynamically stable, identified the 3D structure of metastable-phase crystals, and suggested a new nanoparticle growth mechanism called "multi-stage crystallization." This study holds significance as it reveals a new paradigm in metastable-phase-based material development when most research is focused on developing stable-phase materials.



3D atomic structure of metastable palladium hydride nanoparticles as identified by atomic electron tomography and a schematic of the metastable-phase nanoparticle growth process. Credit: Korea Institute of Science and Technology

Dr. Chun said, "These study findings provide an important process to obtain source technology in the development of advanced alloy materials containing lightweight atoms. An additional study is expected to reveal a new paradigm in the development of metastable-phase-based eco-friendly energy materials that can store hydrogen and lithium. Similar to the Czochralski (CZ) method, which is used to produce single-crystal

silicon, a key material in today's semiconductor industry, it will be a source technology with great potential that will contribute to advanced material development."

More information: Jaeyoung Hong et al, Metastable hexagonal close-packed palladium hydride in liquid cell TEM, *Nature* (2022). [DOI: 10.1038/s41586-021-04391-5](https://doi.org/10.1038/s41586-021-04391-5)

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