Unraveling Metal-to-Metal Hydride Phase Transformation at the Atomic Level Using In Situ Tem Techniques

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Understand metal-to-metal hydride phase transformation at the atomic level using in-situ TEM techniques

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In our quest for a solution to drive the decarbonization of our society and economy, hydrogen shows unique properties as a zero-emission fuel, as an energy storage solution, and as a chemical feedstock. However, compact storage remains a scientific and technological challenge.

Safely storing hydrogen e.g. in the solid form of metal hydrides has many advantages, but further improving its storage properties requires a thorough understanding of the metal to metal hydride phase transformation at the atomic level. Although many techniques have been applied to understand these phase transformations, in-situ visualization of the transformation process with high spatial resolution is essential for a quantitative understanding. For example, stress/strain, defects, and intermediate phase evolution during metal-to-metal hydride phase transformation are crucial to interpret the hydrogen sorption properties.

In this study, we use MgTi thin film as a model system to test, understand, identify and resolve metal-to-metal hydride phase transformation via in situ transmission electron microscopy (TEM). MgTi thin films were prepared via magnetron sputtering, and a focused ion beam (FIB) was used for TEM sample preparation. We observed the Mg to MgH_2 phase transformation by following the bulk plasmon resonance shift in electron energy loss spectroscopy (EELS) and the transition from hexagonal to tetragonal structure by selected area electron diffraction (SAED). Local strain was measured using 4D-STEM, hydrogen atoms in the MgH_2 matrix were identified using integrated differential phase contrast imaging (iDPC). To confirm experimental findings, the accuracy of strain measurement are validated by geometric phase analysis and interpretation of iDPC contrast is supported by image simulation.