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ABSTRACT

Hydrogen in Transition Metal Alloys: Beyond Thermodynamic Limits

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Transition metals readily absorb hydrogen from the gaseous phase, offering high interstitial capacities and mobility, making them attractive for hydrogen storage, purification, sensing, and catalysis. Practical applications demand improvements in storage capacity, kinetics, delivery rates, and reduced formation enthalpies under ambient conditions. Nanostructuring and alloy design provide a means to tailor material properties to meet these demands. We investigate hydrogen absorption mechanisms using well-defined thin films as model systems. Single-crystalline films elucidate strain, finite size effects, and interfaces, while amorphous films provide broad compositional tunability.
To overcome thermodynamic limitations of conventional loading methods relying on thermal energy and pressure, we employ non-equilibrium hydrogen implantation via energetic ion beams, enabling room-temperature exploration of hydrogen concentrations beyond equilibrium limits. The location and concentration of hydrogen are quantified using resonant nuclear reaction analysis (NRA) with high-energy 15N-ion beams, performed at the 5 MV Pelletron Tandem Accelerator at Uppsala University. The ion channeling effect in crystalline materials enables the identification of hydrogen's interstitial sites and vibrational amplitudes by comparing nuclear reaction yields to Monte Carlo simulations. Structural changes in the thin films are analyzed using X-ray reflectivity and diffraction.

As hydrogen is stepwise implantated into thin, single-crystalline V films, the hydride transitions from rom α to β phases onto forming dihydrides. These transtitions are marked by local density fluctuations as phases coexist. For maximally amorphous V_xZr_{1-x} (x = 0.25-0.85) compound systems, we achieve extraordinarily high hydrogen densities varying with composition x. We observe the hydrogen-induced expansion of the amorphous structure and irreversible crystallization as the hydrogen content approaches and exceeds the limit 2 H/M, leading to the formation of new metal hydride phases.