Hydrogen in thin films: controlling stress release paths by microstructure and size

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Metal-hydrogen (M-H) systems offer great opportunities for research studies on fundamental metal systems properties. This is due to the high diffusivity of the smallest of all atoms which allows alloying even at room temperature. When the system size is reduced to the nano-scale, microstructural defects as well as mechanical stress significantly affect the thermodynamics and kinetics properties of the system.[1-6] Effects will be demonstrated on Niobium-H and Palladium-H thin films.
Hydrogen absorption in metal systems commonly leads to lattice expansion. The lateral expansion is hindered when the metal adheres to a rigid substrate, as for thin films. Consequently, high mechanical stresses arise upon hydrogen uptake. In theory, these stresses can reach about -10 GPa for 1 H/M. Usually, metals cannot yield such high stresses and deform plastically. Thereby, maximum compressive mechanical stress of -2 to -3 GPa is commonly measured for 100 nm Nb thin films adhered to Sapphire substrates.
It will be shown that phase transformations change in the coherency state upon film thickness reduction. The coherency state affects the nucleation and growth behaviour of the hydride phase as well as the kinetics of the phase transformation.[1] It will be further demonstrated that plastic deformation can be hindered and even suppressed upon film thickness reduction. In this case the system behaves purely elastic and ultra-high stress of about -10 GPa can be experimentally reached.[2] These high mechanical stresses result in changes of the materials thermodynamics. In the case of Nb-H thin films of less than 8 nm thickness, the common phase transformation from the α-phase solid solution to the hydride phase is completely suppressed, at 300 K.[3,4,5] The stress-conditions can be modulated by using additional lateral confinement [6]. The experimental results go in line with the σDOS model that includes microstructural and mechanical stress effects on the chemical potential [7].

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