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Hydrogen affinity and structural stability of Mg-films on substrates[1] MINA YOON, Oak Ridge National Laboratory, Oak Ridge, MURAT OZER, HANNO WEITERING, University of Tennessee, Knoxville — Using first-principles density functional theory we investigated the binding mechanism of hydrogen to thin Mg films and alloyed films. In ultrathin Mg films the stability of hydrides is much lower than in the corresponding bulk systems and it can be modified by metal alloying. We calculated the chemical potential of hydrogen in Mg films for different dopant species and film thicknesses while including all vibrational degrees of freedom. By comparing the chemical potential with that of free hydrogen gas at finite temperature and pressure, we construct a hydrogenation phase diagram and identify the conditions for hydrogen absorption/desorption. Experimentally those films were synthesized on the Si substrate using MBE technique, where we observed the formation of both Mg and Mg silcides. We studied the competing mechanism of Mg/Mg_2Si formation and their structural stabilities on the substrate.

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