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Interaction of gas-phase hydrogen atom with ultrathin Mg films

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To realize the mobile transportation powered by hydrogen fuel cell, it is needed to develop the small and light hydrogen storage device with large capacity. There have been extensive efforts to achieve ideal hydrogen storage device using metal hydride. However, most of them are not appropriate for practical application because they need high pressure to charge hydrogen and high temperature to discharge. To overcome these problems, it is essential to understand the fundamental processes involved such as the H adsorption, diffusion, and desorption. We have studied the MgH_2 as a model system because of its simplicity and high capacity for hydrogen.

We have investigated the interaction of the gas-phase D atom with an ultrathin Mg film thermally evaporated on SiO_2 by temperature programmed desorption(TPD). MgD_2 is readily formed at room temperature, which upon heating decomposes to simultaneously desorb as D_2 and Mg at 590 K. Decomposition follows a zeroth-order kinetics with an activation energy of 132.5 kJ/mole. The rate of MgD_2 growth is linear with exposure time up to 12 ML with the deuteration probability of 0.6 per incident D atom. The initial growth proceeds via nucleation and growth resulting in a heterogeneous surface layer. 20Å Pd layer deposited on top of deuterated Mg layer acts as an efficient catalyst to greatly reduce the decomposition temperature from 590 to 350 K.