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Origin of anomalous surface lattice expansion in Pd(001)

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We present a systematic study of the hydrogen induced anomalous expansion of the top layer spacing, d12, using low-energy electron diffraction. After exposure of 6 Langmuirs of hydrogen at 150 K sample temperature, the hydrogen atoms occupy the surface hollow sites and a lattice expansion of d12=+4.7 % is determined in agreement with theoretical predictions (5.2 %). Heating the sample above the hydrogen desorption temperature (TD, 340 K), leads to an almost complete relaxation of d12 to the bulk value of 1.945 Å. Similarly, no expansion is observed for clean Pd(001) prepared by rapid cooling after thermal treatment to remove hydrogen. Hydrogen re-adsorption from the residual gas atmosphere and possibly hydrogen agglomeration in the near surface region leads to an expansion of d12 in the 2-3 % range as observed in previous experiments. On the basis of our results, surface magnetism as a mechanism to trigger lattice expansion in Pd(001) needs not to be invoked.