The interaction of water and hydrogen with nickel surfaces

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Stellingen
Behorende bij het proefschrift

The Interaction of Water and Hydrogen with Nickel Surfaces

1. Water can be used as a good titrant for the bare nickel surface area remaining after partial hydrogen adsorption. (this thesis)
2. Sha *et al.* stated that the resurfacing H from a NiH_x layer releases only 0.6 eV energy. This statement disregards the possible occurrence of a phase transition during the decomposition of NiH_x patches, and is therefore incorrect. (Sha X. *et al*, Chem. Phys. Lett. 2002, 357, 389-396 / this thesis)
3. The upward relaxation of certain patches of a thin nickel hydride layer on Ni(111) is hard to detect by or even invisible to LEED measurements. (this thesis)
4. The mechanism proposed by Maynard *et al.* for collision-induced absorption of adsorbed H atoms by impacting noble gas atoms also applies for "D on H" collisions. (Maynard J. K. *et al*, Faraday Discuss. 1991, 91, 437-449 / this thesis)
5. Nakamura *et al.* stated that adsorbed water molecules decompose to yield OD species on Ni(111) at temperatures higher than 165 K. This statement does not consider the influence of remaining water and is therefore misleading. (Nakamura M. *et al*, Chem. Phys. Lett. 2004, 384, 256-261)
6. Schulze *et al.* stated that the TPD feature from ~180 K to ~ 240 K of water when co-adsorbed with oxygen on Ni(111) results from varying water bond energies and differing water-water interactions. This statement is incorrect. (Schulze M. *et al*, J. Anal. Chem. 1995, 353, 661-665)
7. Henkelman *et al.* concluded that for resurfacing of H located underneath a surface-bound species on Ni(111), the surface species either moves out of the way, or the subsurface H hops to adjacent subsurface sites before hopping out into a vacant surface site. To reach this conclusion these authors did not consider all relevant possibilities. (Henkelman G. *et al*, J. Chem. Phys. 2006, 124, 044706)
8. It is difficult to identify water clusters by spectroscopic means only, as evidenced by discrepancies in vibrational mode assignments by the different groups. Because of its atomic resolution capability, STM can help resolve such discrepancies and can provide detailed information about the structure and dynamics of adsorbed water. (Mitsui T. *et al*, Science 2002 297, 1850-1852)
9. The rapid development of computer power and computational methods will result in the replacement of many experimental measurements by computer simulations.
10. It's not about how much you give, it's about how little you expect back.

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Leiden, 15 October 2009