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Formation of cobalt hydrides in low temperature field evaporation

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Abstract

In the field evaporation process of cobalt in an atmosphere of hydrogen 10^{-6} Pa at a temperature of 20 K, both the ions of cobalt and the ones of CoH_x (where x = 1, 2 and 3) have been observed. Since cobalt hydride is typically produced in the direct reaction of cobalt with hydrogen under a pressure of 5 GPa at 600 K, the result of this experiment, which has been carried out under so different conditions, points to the possibility to apply quite a different method of obtaining hydrides of transition metals. The possibility to synthesize such compounds on the surface of cobalt in the high electric field is analysed thanks to quantum chemical methods of calculation (the density functional theory – DFT). Calculated is the equilibrium geometry, the binding energy, and the ionization potential of the cobalt-hydrogen complexes recorded in the experiment. Basing on the computed values and on the measurement of the desorption ions energy distribution, the bond energy of the complexes with the surface has been calculated. Also, the activation energy of filling tetrahedral and octahedral interstices by hydrogen has been determined. Concluding assertion is that the high electric field present at the surface of cobalt during the field desorption process may be the crucial agent that is responsible for the formation of cobalt hydride at the surface.