Preview of abstract after formatting.

Title: Calorimetric investigation of high-pressure nickel hydride
Topic: Materials
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A large hysteresis between the hydride formation (Pf) and decomposition (Pd) pressures is typical of many metal-hydrogen systems. This hysteresis impedes an accurate determination of the equilibrium pressure (Peq). It is widely believed that Peq is much closer to Pd than to Pf, and such an assumption has found a plausible explanation recently (1). However, when the hysteresis is very large (say, about a gigapascal or more) the instruction “much closer” is not very helpful in numerical estimates. Besides, the experimental accuracy in the determination of Pd is usually insufficient for a reliable estimation of the thermodynamical parameters of the hydride formation, because these parameters are very sensitive to the value of Peq due to the large volume effect of the reaction. On the other hand, the same sensitivity can play a positive role and allows one to accurately determine Peq using rather approximate values of the thermodynamical parameters.

In the present paper, we measured the heat of decomposition of a high-pressure hydride NiH using differential scanning calorimetry. A 99.98% nickel foil 0.2 mm thick was loaded with hydrogen at a pressure of 6 GPa and a temperature of 300°C and then cooled to 100 K to avoid hydrogen losses from the synthesized homogeneous NiH samples after the pressure release. Each sample was further sealed in a specially designed capsule preventing losses of the hydrogen gas evolved from the sample in the course of its heating in the calorimeter at a rate of 20°C/min. The measured heat release corresponded to the standard enthalpy $\Delta H0(25°C) = –6.4$ kJ/g-atom H for the reaction $Ni + (1/2)H2 \rightarrow NiH$.

This value significantly differs from the result $\Delta H0(25°C) = –4.2$ kJ/g-atom H of a earlier calorimetric study of decomposition of Ni-H samples prepared using electrochemical techniques. The Peq(T) line calculated using our value of $\Delta H0(25°C)$ well fits the experimental decomposition line of nickel hydride in the whole studied temperature interval from 25°C to the critical point at 360°C (a T-P phase diagram of the Ni-H system gathering together all available experimental results is presented in ref. (3)).

(1) V.E. Antonov, A. I. LatyninandM. Tkacz; J. Phys.: Condens. Matter 16 (2004) 8387.

(2) B. Baranowski, Ber. Bunsensges. physik. Chem. 76 (1972) 714.

(3) V.E. Antonov, A.S. Ivanov, M.A. Kuzovnikov, M. Tkacz, J. Alloys Comp. (2013), http://dx.doi.org/10.1016/j.jallcom.2013.03.021