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NEAR-SOLVUS KINETICS OF HYDROGEN ABSORPTION IN METALS

Solid state hydrogen storage is currently the main alternative to the expensive and hazardous liquefaction technologies. Palladium-based alloys have long been known to absorb prodigious amounts of hydrogen and to possess the necessary catalytic properties. While there is an exhaustive and repeatable data on *thermodynamic* properties of various metal hydrides, certain aspects of absorption *kinetics* remain unclear. The way the attractive H–H interaction and the presence of a two-phase region in the hydride phase diagram affect various kinetic scenarios of hydrogenation has not yet been fully investigated. Mathematical description of hydrogenation accompanied by the first-order phase transition involves insurmountable fundamental difficulties connected with the non-monotonic decrease of thermodynamic potential and hence with inability to write down the governing differential equation for concentration. On the contrary kinetic paths which lie within the single phase region allow application of the standard mathematical tools of the theory of diffusion. In the present work we adopt phenomenological approach to address the effect of attractive hydrogen-hydrogen interaction on hydrogen absorption kinetics in metals under preserved homogeneity of the interstitial solid solution thus formed. A number of peculiar near-solvus kinetic effects are predicted. Numerical solution of the obtained diffusion equation is indicative of a possible multi-stage course of absorption. Hydrogenation rate is shown to slow down in the vicinity of the two-phase region boundary. Predictions of the model are corroborated by the experimental literature data.

Keywords: hydrogen absorption in metals, non-ideal solution, solubility limit, absorption slowdown

Fig. 1. Temporal evolution of radial distribution of absorbed hydrogen concentration in a spherical monocrystalline sample under the reduced temperature value $\theta = 1.1$ (*a*) and $\theta = 1.0001$ (*b*): *a*: $1 - \tau = 0.06, 2 - 0.26, 3 - 0.66, 4 - 1.06$; *b*: $1 - \tau = 0.06, 2 - 1.73, 3 - 2.4, 4 - 3.33, 5 - 4$

Fig. 2. Cumulative absorption curves for the reduced temperature values θ : $1 - 1, 2 = 1.0001, 3 - 1.0004, 4 - 1.1$