Theoretical analysis of reverse hydrogen-induced diffusive phase transformation kinetics in $Nd_{15}Fe_{77}B_8$ alloy

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Kinetics of the hydrogen induced reverse phase transformation in $Nd_{15}Fe_{77}B_8$ alloy at isothermal conditions was described. In terms of the Kolmogrov-Lyubov theory the kinetic diagram of this transformation was calculated. It is shown that kinetics of a reverse phase transformation is controlled by diffusion of Fe atoms in α-Fe matrix.

Описана кинетика индуцированного водородом обратного фазового превращения в сплаве $Nd_{15}Fe_{77}B_8$ в изотермических условиях. На основе теории Колмогорова-Любова рассчитана кинетическая диаграмма этого превращения. Показано, что кинетика обратного фазового превращения контролируется диффузией атомов Fe в матрице α-Fe.

Studies of phase transformation have always been one of the main standpoint areas of solid state physics, metal science, theoretical and practical materials science [1, 2]. The HDDR-process (hydrogenation-decomposition-desorption-recombination) developed recently is based on direct and reverse hydrogen-induced phase transformation in hard magnetic alloy of $Nd_2Fe_{14}B$ type [3]. This process allows to produce permanent magnets from these alloys with improved magnetic characteristics. In [4], the isothermal kinetic diagram of the hydrogen-induced reverse phase transformation in $Nd_{15}Fe_{77}B_8$ alloy was obtained experimentally. Today, however, there is no theory describing such phase transformation. The aim of this work is to describe the above-mentioned isothermal kinetic diagram theoretically using the Kolmogorov-Lyubov kinetic theory of phase transformation.

In hydrogen atmosphere, the hydrogen-induced direct phase transformation (decomposition) in $Nd_2Fe_{14}B$ alloy occurs according to the following scheme [3]:

$$Nd_2Fe_{14}B \rightarrow NdH_2 + 12\alpha\text{–}Fe + Fe_2B. \quad (1)$$

The reverse phase transformation (recombination) in $Nd_2Fe_{14}B$ alloy occurs in vacuum according to the following scheme [3]:

$$NdH_2 + 12\alpha\text{–}Fe + Fe_2B \rightarrow Nd_2Fe_{14}B. \quad (2)$$

Isothermal kinetic diagram for hydrogen-induced reverse phase transformation in $Nd_{15}Fe_{77}B_8$ (at. %) alloy was obtained in [4] by magnetometric measurements. This diagram is shown in Fig. 1. Basing on kinetic investigations [4, 5] and electron microscopy and X-ray diffraction studies [6] of the reverse phase transformation in $Nd_2Fe_{14}B$ type alloys, it was shown before that transformations of this type is a diffusive phase one in solid state and that the reverse transformation proceeds be the nucleation and growth mechanism.

As follows from Becker-Doering theory [7], plotting the dependence $\ln t_\xi$ on $1/T$, where t_ξ is the time required to attain a certain transformation degree ξ and T is the temperature, we can determine the effective energy of phase transformation process. To that end, the experimental data from Fig. 1 were re-plotted in $\ln t_\xi$ vs. $1/T$ co-ordinates (Fig. 2). Thus, the slopes of the straight