

THE PECULIARITIES OF Ti INTERACTION WITH ATOMIC HYDROGEN

Matysina Z.A.*, Zaginaichenko S.Yu., Schur D.V.

Institute for Problems of Materials Science of NAS of Ukraine, Laboratory №67,
3 Krzhyzhanovsky str., Kyiv, 03142 Ukraine

* Fax: 38 (044) 424-0381, E-mail: shurzag@materials.kiev.ua

Introduction

The use of nuclear reactors in a hydrogen cycle supposes their safe operation. An important condition for this operation is to possess the information about the processes proceeding in the bulk of materials from which construction elements of a reactor are made.

Therefore the theoretical research into phase transformations in titanium during its interaction with hydrogen is of high importance.

Based on the molecular-kinetic theory, this work considers thermo-dynamical conditions for phase transformations in titanium that occur during its interaction with hydrogen.

Result of discussions

This work presents the study of phase transitions of $\alpha \rightarrow \beta \rightarrow \gamma$ type observed in titanium over the temperature region 573-1073K. For this purpose the free energies of phases are calculated, their concentrational dependence is estimated, the conditions of possible each phase realization are established and the constitution diagram is constructed using the plots of concentrational dependences of phases free energies at different temperatures and theoretical diagram is in agreement with experimental in a qualitative sense for titanium hydride.

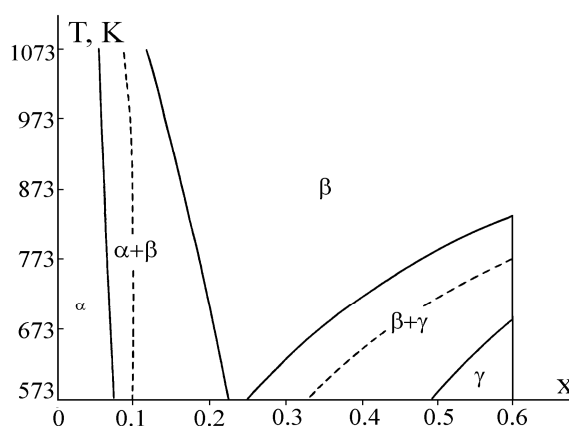
The calculation of free energies has been carried out using molecular-kinetic theory on the assumption of geometrical ideality of crystal lattices and taking into consideration the interatomic interactions for the nearest pairs and also the presence of atomic order in arrangement of hydrogen atoms at the tetrahedral and octahedral interstitial sites.

The terms that depend on the energies of interaction of hydrogen atoms and metal atoms and between one another and on the character of hydrogen atoms distribution at tetrahedral and octahedral interstitial sites are considered. The interstitial sites are taken as those of the first and the second type, respectively. In this case the tetrahedral interstitial sites will be valid for hydrogen atoms.

From Fig. we notice that: 1) the concentrational range of α phase existence is constricted slightly with increasing temperature, 2) the concentrational ranges of two phases $\alpha + \beta$ and phases $\beta + \gamma$ are constricted also with increase in temperature, 3) the concentrational range of β phase existence increases considerably with a rise in temperature, 4) the γ phase exist in a small temperature and concentration intervals. In this case the γ phase is not stable, because in the considered interval of concentrations the free

energy $f_\gamma(x)$ has no minimum, which corresponds to equilibrium state of system. For this reason the γ phase was not always made evident experimentally. The occurrence of γ phase has been noted in papers.

Fig. Theoretical constitution diagram of Ti-H system, constructed by the intersection points of the free energies plots and by points of common tangent lines to these curves. The full curves, constructed by points of common tangent lines to the $f_\alpha(x)$, $f_\beta(x)$, $f_\gamma(x)$ curves, determine the phase diagram with consideration for two-phase existence of system state. The dotted curves, constructed by points of intersection of the $f_\alpha(x)$, $f_\beta(x)$ and $f_\beta(x)$, $f_\gamma(x)$ curves, define the phase diagram without considering two-phase existence of system regions.



Conclusions

Thus, the statistic theory of metals and alloys allows to explain and substantiate the solid-phase transformations accompanied with the change of crystal lattice structure and permits to make an estimate of phase transformations temperatures.

The theory developed allow evaluation of the concentrational intervals of α, β, γ phases existence in the alloy Ti-H, explanation of the change regularities of concentrational intervals for these phases with variation in temperature. In this case the theoretical constitution diagram is in qualitative agreement with experimental diagram for titanium hydride.

All mentioned regularities are in agreement with experimental data on the construction of constitution diagram of titanium-hydrogen system.

Acknowledgment

The work has been performed under support of

Science and Technology Center in Ukraine,
Project # Uzb-131.