HYDROGEN BICOMPLEXES AND INTERSTITIAL CROWDIONS INSIDE CRYSTALS. HYDROGEN SOLUBILITY

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In case of high concentration of hydrogen in the crystals (e.g. in accumu1ators) it could appear energetically advantageous the hydrogen atoms distribution in interstitial sites of different types, e.g. octahedral, tetrahedral, triangular as well as in sites of crystal lattice and as a consequence the forming of thermodynamically equilibrium hydrogen complexes such as dumb-bells of various type, linear and flat triple and quadruple complexes, crowdions. The binary disordered al1oy with face-centered cubic lattice has been studied. Calculations has been carried out on basis of molecular-kinetic theory in simplified model of crystal. It is assumed that crystal lattice is geometrically ideal. Atoms interaction has been taken into consideration in the first coordinational sphere. Relaxation of lattice and correlation in replacement of sites and interstitial sites by corresponding atoms are not taken into account.

An energetic advantageous of hydrogen complexes creation has been justified. Hydrogen solubility has been calculated taking into consideration the complexes creation and plots of hydrogen solubility dependence on temperature has been constructed. It has been shown that creation of hydrogen complexes increases the hydrogen solubi1ity.

Theoretical results have been compared with experimental data hydrogen solubility in alloys Fe-Ni, Fe-V, Pd-Ni and Pd-Pt.

References

1. Schur DV, Zaginaichenko SYu, Adejev VM, Voitovich VB, Lyashenko AA, Trefilov VI, Phase transformations in titanium hydrides, International journal of hydrogen energy, 21, 11, 1121-1124, 1996, Pergamon

2. Matysina ZA, Pogorelova OS, Zaginaichenko SYu, Schur DV, The surface energy of crystalline CuZn and FeAl alloys, Journal of Physics and Chemistry of Solids, 56, 1, 9-14, 1995, Elsevier

3. Isayev KB, Schur DV, Study of thermophysical properties of a metal-hydrogen system, International journal of hydrogen energy, 21, 11, 1129-1132, 1996, Pergamon

4. Schur DV, Lavrenko VA, Adejev VM, Kirjakova IE, Studies of the hydride formation mechanism in metals, International journal of hydrogen energy, 19, 3, 265-268, 1994, Elsevier

5. Matysina ZA, Zaginaichenko SYu, Schur DV, Hydrogen solubility in alloys under pressure, International journal of hydrogen energy, 21, 11, 1085-1089, 1996, Pergamon

6. Schur DV, Lyashenko AA, Adejev VM, Voitovich VB, Zaginaichenko S Yu, Niobium as a construction material for a hydrogen energy system, International journal of hydrogen energy, 20, 5, 405-407, 1995, Elsevier