THE MUTUAL INFLUENCE OF INTERSTITIAL IMPURITIES IN ALLOYS WITH STRUCTURE OF IRON BORIDE TYPE

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The alloying of metals and alloys with different interstitial impurities permits the considerable regulation of their properties at the expense of these interstitial additions. On evidence of experimental investigations hydrogen solubility versus silicon, boron and carbon concentration in Ni, Pd and Fe manifests itself variously, i.e. one of the interstitial impurities can both to inhibit the solubility of another and to favour it.

In present research work the theoretical investigation of hydrogen, carbon and other elements solubility in alloys of $(RD)_2$ GS type with the structure of iron boride Fe_2B type has been performed. In studied phases the R, D metals atoms can be Fe, Co, Ni, Cr, Mn, Mo, Au, Al, To, Ta, W, Zr atoms and others, the G, S non-metals atoms - H, C, B, P, Ge, Si, Sn atoms and others. The Shubert and modified Yum-Rozeri models of iron boride structure has been used. The free energy of interstitial alloys has been calculated without taking into account the correlation in atoms distribution by configurational method taking into consideration the configurations of R, D metals atoms around the G, S atoms. The atomic order in distribution of R, D atoms over sites and of G, S atoms over interstitial sites is not taken into consideration. The interaction between nearest atomic pair G, S and with R, D metal atoms is taken into account.

Authors have received formulae determining the hydrogen, carbon solubility in alloy in dependence on temperature, concentrations of R, D components and energetic constants and also defining the mutual influence of hydrogen and carbon solubility in alloy. The obtained formulae admits the presence of extremum at the temperature dependence of solubility of these elements. It has been found that interstitial impurities are favourable for the dissolution each other in alloy at their atoms interaction of attraction type, and vice versa these impurities inhibit the dissolution each other in the case of repulsion forces between atoms. At the investigation of carbon and boron solubility in iron boride the obtained dependences are in agreement with experimental data according to which the boron presence in alloy decrease the carbon solubility.

The obtained theoretical formulae on mutual influence of one interstitial impurity solubility on another are in agreement with experimental results of effect of silicon, boron, carbon on hydrogen solubility.

References

1. Isayev KB, Schur DV, Study of thermophysical properties of a metal-hydrogen system, International journal of hydrogen energy, 21, 11, 1129-1132, 1996, Pergamon
2. Matysina ZA, Zaginaichenko SYu, Schur DV, Hydrogen solubility in alloys under pressure, International journal of hydrogen energy, 21, 11, 1085-1089, 1996, Pergamon
3. 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
4. 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
5. 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