INTERACTION IN $CeCo_{2.95}M_{0.05}$-H_2 (M-Cu, Si) SYSTEM UNDER HYDROGEN PRESSURE UP TO 100 atm

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Introduction

Intermetallic compounds RT_3 form stable hydride phases with reversibly hydrogen desorption and can be used for practical applications as materials for storage hydrogen. Interaction of RT_3 intermetallic compounds (R-earth element of Ce subgroup, T-Ni, Co) with hydrogen leads to forming hydride phases containing about 1.5 mass % of hydrogen [1]. For example, in $CeCo_3$-H_2 system hydrogen desorption pressure is 0.5 atm at 75^0C and this make possibility to use alloys based on $CeCo_3$ for storage hydrogen. Thermal stability and equilibrium pressure of dissociation are important properties of hydride phase for practical application. Introduction of different metals in $CeCo_3$ composition allows change these properties of hydride phase's formed in IMC-hydrogen system. At present work interaction of $CeCo_{2.95}M_{0.05}$, (M-Cu, Si) with hydrogen under pressure up to100 atm. have been studied.

Results and disscusion

Samples of $CeCo_{2.95}Cu_{0.05}$ and $CeCo_{2.95}Si_{0.05}$ were melted in electric furnace under inert atmosphere and after that quenched during 240 hours at 950^0C. Synthesis of hydrides and equilibrium pressure study were carried out at Sivert's apparatus under hydrogen pressure up to 100 atm. For work was used pure hydrogen out of hydride storage device with alloy based on $LaNi_5$. Investigation in IMC-hydrogen system have been carried out with pressure-composition isotherms measuring. Hydrides were obtained using «soft» method of synthesis. In this case hydrogen was delivered with pieces under small pressure until hydride phase full saturation. This method allows avoiding of forming amorphous products of reaction. X-ray diffraction data were obtained at DRON-2 diffractometr.

X-ray analyses of obtained alloy samples revealed that they were single-phases. Measured desorption isotherms in $CeCo_{2.95}Cu_{0.05}$-H_2 system at 50^0C, 75^0C and 99^0C temperatures showed presence of two phases close to $CeCo_{2.95}Cu_{0.05}H_3$ and $CeCo_{2.95}Cu_{0.05}H_4$ composition as was established early in [1] for $CeCo_3$-H_2 system. Small decreasing of equilibrium pressure of dissociation in comparison with $CeCo_3$-H_2 system demonstrated that Cu introduction in alloy increased hydride phases stability. In case of $CeCo_{2.95}Si_{0.05}$ sample it was contrary result – in IMC-hydrogen system equilibrium pressure of hydride phases decomposition increased. Measured isotherms at 50^0C, 75^0C and 99^0C temperatures showed presence of three phases with $CeCo_{2.95}Si_{0.05}H_2$, $CeCo_{2.95}Si_{0.05}H_3$ and $CeCo_{2.95}Si_{0.05}H_4$ composition.

Such behaviour during decomposition of hydrides based on $CeCo_3$ compound containing Si with large atomic radius probably occurs for the reason that the volume of vacancies in lattice was increased. This leads to weak bonds between hydrogen and metallic atoms surrounding vacancies and for forming hydride phase it is necessary increase pressure of hydrogen. In case of Cu introduced in alloy close chemistry properties and size of Cu and Co not caused any substantial influence on the properties of synthesised hydride phases.

As a result Si introduction leads to increasing of equilibrium pressure of dissociation of formed hydride phases in comparison with $CeCo_3$-H_2 system without their remarkable changing of hydrogen content.

Using obtained data of equilibrium pressure of dissociation in $CeCo_{2.95}M_{0.05}$-H_2 (M-Cu, Si) system an enthalpy of the phases transitions have been calculated. Obtained data showed that enthalpy of hydride phases formed in $CeCo_{2.95}Cu_{0.05}$-H_2 and $CeCo_3$-H_2 systems were practically in coincidence. In $CeCo_{2.95}Si_{0.05}$-H_2 system enthalpy of hydrides forming was less than for hydrides of $CeCo_3$-H_2 system.

X-ray data of synthesized hydrides showed that they have hexagonal anisotropic lattice of initial intermetallic with increased *c* parameter.

Conclusions

Interaction in $CeCo_{2.95}M_{0.05}$-H_2 (M-Cu, Si) systems under hydrogen pressure up to 100 atm has been studied with measurement pressure composition isotherms. Equilibrium pressure of hydride phase's dissociation and their

thermodynamic function were determinate. Hydrogen content in synthesised hydrides are correspond to quantity hydrogen in hydrides base d on $CeCo_3$ compound. X-ray data revealed that formed hydrides have anisotropic expanded lattice with symmetry of initial alloys.

References

1. Burnasheva V.V., Klimeshin V.V., Semenenko K.N. Study equilibrium in RCo_3-H_2 systems, where R-Ce, Pr, Tb, Dy and Er. Inorg. Mat.1979:15(2): 251-255.