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Interacting lattice gas model for hydrogen subsystem of metal hydrides

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Thermodynamic behavior of hydrogen subsystem in Me-H interstitial solid solutions has been analyzed. A model of interacting lattice gas has been proposed taking account for both direct atomic interaction and the lattice dilatation at hydrogen dissolution. The molecular H_2 phase in equilibrium with the metal hydride and the lattice gas consisting of H atoms have been described using an original scheme of thermodynamic perturbation theory. The contributions due to attraction energy have been concluded to play the decisive part in equilibrium properties of the hydrogen component in Me-H solutions.

Описание особенностей PCT-диаграмм металлогидридов требует анализа термодинамического поведения водородной подсистемы растворов внедрения М-Г. Предложена модель неидеального (взаимодействующего) решеточного газа с учетом прямого межатомного взаимодействия и расширения решетки при растворении водорода. Термодинамическое описание молекулярной фазы H_2, равновесной с металлогидридом, и решеточного газа Н-атомов проведено на базе оригинальной схемы термодинамической теории возмущений. Сделан вывод об определяющей роли вкладов, обусловленных энергией притяжения, в равновесные свойства водородного компонента растворов М-Г.

The lattice gas model for hydrogen component of metal hydrides (MH) considers the phase transitions associated with redistribution of H atoms in metal matrix of interstitial solutions as changes in aggregate state of "lattice fluid" [1–3]. For example, a solid solution decomposition into two disordered phases of different concentrations answers to the gas-to-liquid phase transition (the lattice gas condensation). Besides of proper phase equilibria (PCT diagrams), of considerable interest are, in particular, parameters of phase transition critical points in hydrides being used as working media in heat sorption compressors, heat pumps, hydrogen storage systems, hydrogen isotopes separation devices, etc. [1].

Our study is aimed at the description of observed phase transition peculiarities in transition metal hydrides of practical importance. The work states the principles of a novel approach to the problem consisting in determination of thermodynamic properties for non-ideal hydrogen subsystem of MH in the frame of the unified modified perturbation theory (MPT) scheme [4]. The critical parameters of phase transitions under consideration are rather easy to determine within the MPT scheme and are of a considerable information value for modeling the atomic H-H interaction character in the lattice gas.

In fact, at the level of estimation, the critical temperature T_c of the gas-liquid phase transition is in a proportion to a