Structure Transformations in the Saturated Hydrides $ZrV_2H_{4<x<6}$

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We have studied, by means of neutron powder diffraction, the structure transformations caused by hydrogen redistributions in the Laves saturated hydrides ZrV_2H_x, $4<x<6$. In the range of $4<x<5$, the uncommon order-disorder phase transition has been found [1]. Unlike the known transitions in the unsaturated hydrides, $x<4$, it results in change of hydrogen surroundings when hydrogen ordering. As a result, the novel hydrogen superstructure ZrV_2H_5, with the atypical hydrogen surroundings, forms [2]. At maximum hydrogen saturation, near $x=6$, whatever phase transitions are eliminated. The maximum hydride ZrV_2H_6 exists only as ordered, and any attempt to disarrange the hydrogen results in hydrogen discharge down to $x=5$. The crystal structure of ZrV_2H_6 has been determined [3]. It is advance of the Spinel-type structure found earlier in the saturated hydrides $ZrTi_2H_4$ and $HfTi_2H_4$. The work was partly supported by the Russian Foundation for Basic Research and Russian State Program HIII-2037.2003.2.

[1] Bogdanova A.N., Andre G., *J. Alloys Comp*., 2004, **379**, 54. [2] Bogdanova A.N., Irodova A.V., Andre G., Bouree F., *J. Alloys Comp*., *in press*. [3] Bogdanova A.N., Irodova A.V., Andre G., Bouree F., *J. Alloys Comp.*, 2003, **50**, 356-357.

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