

STRUCTURE OF NbVCoD_{2,3}, SYNTEZIED UNDER HIGH GASEOUS PRESSURE (UP TO 2000 ATM.)

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Introduction

IMC AB₂ with Laves structure are promising materials for storage hydrogen. Under usual pressures (up to 100 atm.) hydride phases in AB₂-H₂ system able to absorb until two mass percent of hydrogen. IMC NbVCo is unusual, the interaction with hydrogen doesn't occurred under low pressure (up to 100 atm.) and room temperature [1]. Using of high pressure of hydrogen (up to 2000 atm.) allowed to obtain hydride phase with amount hydrogen 3,0 H/IMC.

For determination of site hydrogen atoms in synthesized hydride neutron powder diffraction study has been performed.

Results and discussion

After synthesis of deuteride maximum amount of deuterium equally NbVCoD_{2,5} has been measured with thermodesorption method.

X-ray analyses of NbVCoD_{2,5} has been revealed that obtained hydride phase remain structure of initial compound with increased lattice parameters.

Position of metal and deuterium atoms has been determined by X-ray and neutron powder diffraction.

Has been demonstrated that V and Co atoms distributed in B-component sublattice (2a, 6h) and deuterium atoms mainly occupied 24l and 12k sites. Deuterium amount obtained from neutron data NbVCoD_{2,3} is a bit less than in synthesized deuteride.

Summary

Using of high deuterium pressure allowed perform synthesis of deuteride NbVCoD_{2,3}. Obtained distribution of deuterium atoms revealed usual for Laves phases.

References

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