NEUTRON DIFFRACTION STUDY OF ISOTOPIC EFFECT IN ARRANGEMENT OF HYDROGEN ATOMS IN SOLID SOLUTIONS OF SYSTEM Ti-N-H (D)

I. KHIDIROV, N. N. MUKHTAROVA
Institute of Nuclear Physics, Uzbekistan Academy of Sciences, Tashkent, Uzbekistan

Neutron diffraction and X-ray diffraction were applied to study the ordering in the $TiN_{0,26}H_{0,15}$, $TiN_{0.26}D_{0.15}$ and $TiN_{0.40}H_{0.19}D_{0.19}$ solid solutions. Hydrogen atoms are found to redistribute over octahedral and tetrahedral interstices of the hexagonal close-packed structure of the $TiN_{0.26}H_{0.15}$ solid solution with varying temperature. Consecutive ordering-decay processes and the ordering of antiphase domains are discovered at temperatures below the decay temperature. In a high-temperature disordered state, isotopically different solid solutions $TiN_{0.26}H_{0.15}$, $TiN_{0.26}D_{0.15}$ have identical structural characteristics; as temperature decreases, an isotopic effect comes into operation. This effect consists of the following: as opposed to the hydrogen solid solution, in the deuterium solid solution ordering starts at a far higher temperature; an ordered monoclinic phase has a larger homogeneous region; interstitial ^2D and ^1H distribution over interstices is different in character; and the blocking effect between interstitial atoms is more pronounced. The displacement

of hydrogen atoms from the center of the tetrahedron along the c axis has different signs in the disordered and ordered solid solutions.

By neutron structure analysis the crystal structure of the solid solution with the combined isotope composition on the base of titanium - $TiN_{0.40}H_{0.19}D_{0.19}$ was studied (space group $D\bar{3}m1$). It was found isotopic effect in distribution of the hydrogen isotopes H and D: the isotopes arrange over the same type of tetrahedral interstices but have different coordinates z, i.e. the splitting of a set of tetrahedral positions 2d into hydrogen (H) and deuterium (D) is observed. It follows that in the ordered «layered» structure of the solid solution $TiN_{0,40}H_{0,19}D_{0,19}$ there can not be two different isotopes of the same element on one plane perpendicular to threefold axis. Crystal-chemistry analysis of environment of H and D is carried out and the essential differences in coordination polyhedrons surrounding the two isotopes are revealed. Analysis of the results shows that in a number of Me-N-D systems hydrogen and deuterium should be considered as independent components.