

Neutron Diffraction Study for Local Analysis of Deuterium Sites in TiZrNi alloy

Sang-Hwa Lee¹, Ashfia Huq² Jaeyong Kim³

¹Neutron Utilization Research Division, Korea Atomic Energy Research Institute, Daejeon, Republic of Korea

²Spallation Neutron Source, Oak Ridge National Laboratory, TN, USA.

³Department of Physics, Hanyang University, Seoul, Korea.

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TiZr-based alloys are known to absorb a large amount of hydrogen, and as such have been proposed as candidate materials for hydrogen storage applications. For the preferential site analysis, as-cast TiZrNi alloys were prepared and partially deuterated using a lab-built isotherm measurement system to locate the atomic positions of host metals with deuterium before evaluating their technical usefulness. Results of Rietveld refinements measured from simultaneous fit of X-ray and neutron diffraction patterns revealed that slowly cooled $\text{Ti}_{53}\text{Zr}_{27}\text{Ni}_{20}$ alloys have a C14 Laves phase (P63/mmc) with lattice constants of $a=5.27$ and $c=8.31$ Å with atomic compositions of 52.25, 28.27 and 19.48 at. % for Ti, Zr, and Ni, respectively. Deuterium atoms sit in tetrahedral sites formed by Ti_2Zr_2 and Zr_2Ni_2 . The exact locations of the deuterium atoms are (0.412, 0.462, 0.594) and (0.430, 0.569, 0.250) of Wyckoff positions in a xyz coordinate system. The formation of a hydride phase was unavoidable even at low concentrations of deuterium, and was identified to TiD_2 .

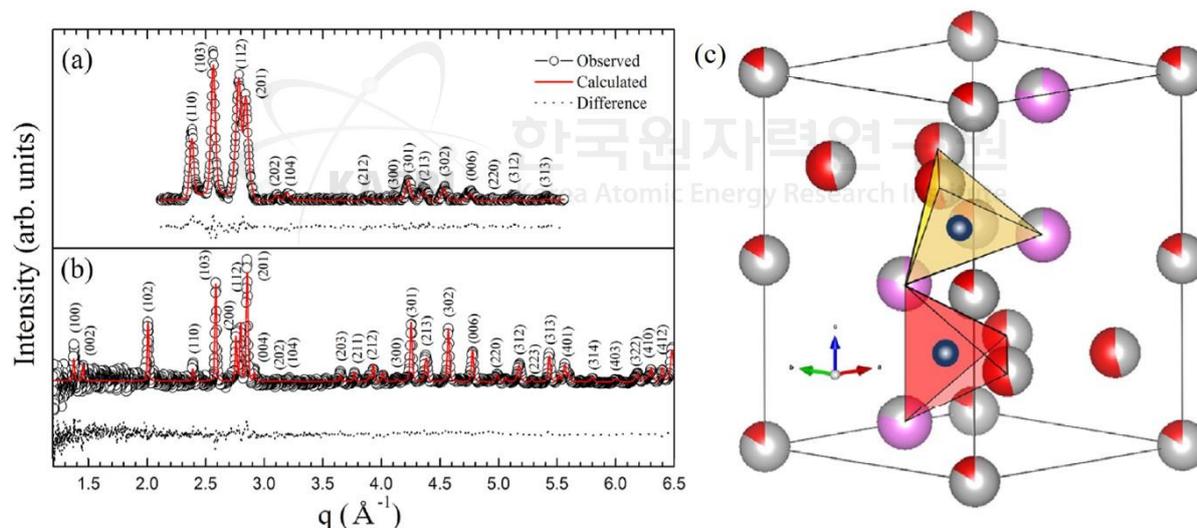


Fig. Results of Rietveld refinements for (a) X-ray and (b) neutron diffraction patterns measured from as-cast $\text{Ti}_{53}\text{Zr}_{27}\text{Ni}_{20}$ alloys. The diffraction data and calculated paesk for C14 phase are shown and solid lines, respectively. (c) Structure modeling of as-cast $\text{Ti}_{53}\text{Zr}_{27}\text{Ni}_{20}$ Laves phase with deuterium positions. Ti, Zr, Ni and D are represented in grey, pink, read and blue, respectively. The fraction of the color of the atom solid lines.

