

In situ Neutron Diffraction on $D_x\text{Nb}_2\text{O}_5$

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$D_x\text{Nb}_2\text{O}_5$ is thermodynamically unstable. Therefore, neutron diffraction measurements were performed in the electrochemical cell used for the intercalation of deuterium into sintered Nb_2O_5 powder samples. Diffraction patterns were recorded at equilibrium potentials of -443 , -428 , -332 and -197 mV vs. NHE (corresponding to $x = 0.232$, $x = 0.23$, $x = 0.21$ and $x = 0.06$). The structural changes in Nb_2O_5 caused by the deuterium insertion are small but could be determined reproducibly. The lattice parameters of the host lattice exhibit a characteristic dependence on the deuterium content of the bronze. A model has been developed for the partially inhomogeneous distribution of the deuterium in the Nb_2O_5 unit cell, which explains the changes of the peak intensities observed in the low angle region ($6^\circ \leq 2\theta \leq 18^\circ$).

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