THE ELECTRONIC AND ELECTROCHEMICAL PROPERTIES OF THE $TiFe$-BASED ALLOYS

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9.7 cm

The titanium compounds TiX ($X = Fe, Co, Ni$), with $CsCl$-type structure are promissing hydrogen storage materials. The capacity of the hydrogen absorption in these compounds is known to be smaller than the value which would be expected from the crystal geometry. The high-energy milling technique is generally used to modify the surface structure and texture of materials in order to improve their physical or chemical properties. In this work we present results for $TiFe_{1-x}Ni_x$ compounds. The electrochemical properties of these materials have been investigated and discharge capacity enhancement has been observed. With increasing nickel content in $TiFe_{1-x}Ni_x$, the material showed an increase in discharge capacity which passed through a maximum for $x = 3/4$. The electronic structure has been studied by the tight binding version of the linear muffin-tin orbital method in the atomic sphere approximation ($TB\ LMTO\ ASA$). A systematic study of electronic structure for $TiFe_{1-x}Ni_x$ alloys will be presented in whole range of concentration from $TiFe$ to $TiNi$ with a step of $\Delta x = 1/8$. The calculations show a coincidence between discharge capacity and calculated characteristics like charge transfer between ions and density of electronic states at the Fermi level.

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