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Electrochemical Hydrogen Insertion into Ti-Zr and Ti-V Carbides

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In the field of hydrogen storage materials, there is a growing need for the development of cheap and effective solutions. Recently it has been shown both experimentally[1][2][3] and theoretically[4] that hydrogen insertion is possible into substoichiometric titanium carbides TiC_x, when the value of x is close to 0.6. Titanium and carbon being abundant and hence low-cost chemical elements, this renders TiC a promising material for hydrogen storage.

In this invited presentation, we show and discuss results of electrochemical hydrogen insertion into substoichiometric carbides, where Ti has been substituted by zirconium (of the same chemical group) or vanadium (the following element in the same period). Materials have been syntesized by reactive hot-press sintering at high temperature (1800 °C, 40 MPa) from commercial powders of TiC and Ti, Zr, and-or V metals. The electrochemical experiments show that hydrogen insertion and extraction is significantly increased when Zr is in substitution of Ti. It is the contrary when V is introduced in the material. These experimental results are confirmed by first-principles calculations. Concerning the Zr-containing material, it is explained by the fact that the Zr-H bond is much weaker than the Ti-H bond, so the diffusivity is increased. For the V-containing material, it is shown that less hydrogen can be inserted in the lattice, and that the formation of the hydrogen-carbon vacancy complex is more difficult.

Keywords: Titanium carbide; Zirconium or vanadium substitution; Substoichiometry; Hydrogen insertion; First-principles calcluations.

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[1] A. Gringoz, N. Glandut, S. Valette, Electrochem. Commun. 11 (2009) 2044-7.
[2] J. Nguyen, N. Glandut, C. Jaoul, P. Lefort, Langmuir 29 (2013) 12036-42.
[3] J. Nguyen, N. Glandut, C. Jaoul, P. Lefort, submitted.
[4] H. Ding, X. Fan, C. Li, X. Liu, D. Jiang, C. Wang, J. Alloys Compd. 551 (2013) 67-71.