

## عنوان مقاله:

Substitution effects on the shape memory and hydrogenation properties of TiNi

## محل انتشار:

سومین کنفرانس هیدروژن و پیل سوختی (سال: 1394)

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## خلاصه مقاله:

This study aims to improve shape memory and hydrogen storage properties of TiNi by chemical substitutions in the Ni sub-lattice. The effect of Pd, Cu and Co substitutions on crystal structure, martensitic transformation and hydrogenation properties of TiNi has been studied by structural (X-ray and neutron powder diffraction), calorimetric, solid-gas and electrochemical means. Ab initio DFT calculations were done to highlight electronic effects on hydrogenation properties. The three substitutions, TiNi<sub>1-z</sub>M<sub>z</sub> (M = Pd, Cu and Co; z ≤ 0.5), lead to the formation of pseudobinary compounds. Substitutions by Pd and Cu increase the unit-cell volume of TiNi, whereas the reverse effect occurs for Co. Martensitic transformation temperatures correlate with volume variations. They increase strongly for M = Pd and slightly for M = Cu, whereas M = Co decreases it. Hydrogenation properties are very sensitive to chemical elements substitution. The capacity decreases strongly for M = Pd, moderately for M = Cu and remains stable for M = Co. Contrary to expected effect by geometric model, both Pd and Cu substitutions decrease the stability of hydrides. DFT calculations show that electronic rather than geometric effects govern hydride stability for M = Pd. Co substitution induces step-wise formation of hydrides with a multi-plateau behaviour in pressure-composition isotherms. As concerns applications, low amount of Cu substitution (z = 0.2) increases the electrochemical discharge capacity of TiNi from 150 to 300 mAh/g due to hydride destabilization. This opens new perspectives for using TiNi-based alloys in Ni-MH batteries. In contrast, Pd and high amount of Cu substitution (z = 0.5) are effective to decrease TiNi reactivity towards hydrogen, and therefore attractive for shape memory applications under reductive environment.

## کلمات کلیدی:

TiNi, pseudo-binary compounds, martensitic transformation, hydrogenation properties, Ni-MH batteries

## لینک ثابت مقاله در پایگاه سیویلیکا:

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