

”Hydrogenation–disordering of structure” correlations for Ni/Co-based nanomaterials

I. Zavaliiy, A. Kytsya, Yu. Verbovytskyy, K. Vlad, V. Berezovets

Karpenko Physico-Mechanical Institute of the NAS of Ukraine. Naukova Str., 5, Lviv-79060, Ukraine

e-mail: ihor.zavaliiy@gmail.com

Ni(Co)-based nanomaterials could be used as effective catalysts for different chemical reactions, where atomic/molecular hydrogen is involved. *E.g.*, they could be used as catalyst for CO₂ methanation [1] or for the effective generation of hydrogen by hydrolysis of NaBH₄ [2]. At the same time, it is known that Co-based nanopowders possess high electrochemical discharge capacity [3]. However, despite the long history of the investigation of the hydrogenation of nickel, the nature of hydrogen absorption by the nickel-based nanomaterials is still debatable [3]. The question about the correlation of catalytic and hydrogenation properties is also opened. The aim of this report will be the overview of the relationships between the structure of mono Ni(Co) and bimetallic Ni/Co nanostructured powders and their hydrogenation properties.

Mono Ni(Co) and bimetallic Ni/Co nanostructured powders were synthesized by chemical reduction and by leaching of Al from the Ni/Co/Al alloys at different ratios of elements. The structure of the obtained nanopowders was carefully investigated using SEM, TEM, HRTEM, XRD, SAXS and low-temperature gas adsorption techniques. Electrochemical and gas hydrogenation of obtained nanomaterials were investigated also by the different techniques.

It was found that majority of the studied samples were characterized by substantial discharge capacity despite the quit low porosity of the powders. For example, despite the low porosity, the Nickel-leached as well Ni-NPs (obtained by chemical reduction) were characterized by discharge capacity in the range 10–150 mAh/g. This fact was clarified by the precisions investigations of the structure. Thus, the size of Ni particles, obtained by the different methods, was within range 10–100 nm. The results of HRTEM indicates the mono- or polycrystalline nature of the samples with the size of crystallites (calculated by XRD patterns) in the range 5–90 nm. The detailed analysis of SAXS patterns indicates the presence of inhomogeneities with the size of 6–10 Å for the Ni nanopowders. Such inhomogeneities are caused by the diffusive borders between the crystallites and are too small for the diffusion of the nitrogen but are enough for the permeability and/or absorption of hydrogen. The analysis of the dependence of hydrogenation properties on “the disordering of structure” will be done for the nanopowders with different crystallite size as well as for amorphous samples. The relationships between the structure of Ni and Ni-Co nanopowders and observed hydrogenation properties will be analyzed also on the dependence of the Ni/Co ratio.

[1] P. Shafiee, S. Alavi, M. Rezaei, *et al. Int. J. Hydrogen Energy*, 47/4, (2022) 2399-2411. <https://doi.org/10.1016/j.ijhydene.2021.10.197>

[2] A. Kytsya, V. Berezovets, Yu. Verbovytskyy, *et al. J. Alloys Comp.*, 908 (2022) 164484. <https://doi.org/10.1016/j.jallcom.2022.164484>

[3] Liu Y, Wang Y, Xiao L, *et al Electrochem Commun* 9/5 (2007) 925-929. <https://doi.org/10.1016/j.elecom.2006.11.034>

[4] I. Marchuck, T. Zasadnyy, I. Zavaliiy. *Physico-Chemical Mechanics of Materials (Ukr.. transl. to Engl. as Mat. Sci.)*, 6 (2024) 6-15.