Semester report

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PhD program: Materials science and solid state physics

Supervisor: Révész Ádám

Thesis title: Hydrogen storage of non-equilibrium materials

Introduction:

Continuous population and development growth lead to increased energy consumption. Most of modern energy sources are non-renewable and resulting in CO_2 or other greenhouse gases emission. Nevertheless, renewable energy sources attract more and more attention due to environmental reasons, global warming in particular. One of renewable sources the major downside is unpredictability, wind turbines can show maximal output at midnight, but they can stop at morning when consumption peak appears. Other significant problem is transportation, renewable sources usually geographically bonded to certain regions which can be remote relative to the consumption centers. Solution for these issues contains unavoidable energy storage step. One of the most promising energy storage solution is hydrogen. This molecular gas can be simply obtained from water by electrolysis and efficiently transformed back into water and energy by means of fuel cells without harmful by-products. There are 3 main storage forms for hydrogen: gas, liquid and solid. igh pressure is needed to store a sufficient amount of hydrogen in gaseous form, liquid form provides a higher energy density but requires high energy input to reduce the temperature. Relatively low energy density and high explosion risks create barrier for production of mobile storage units. Solid phase storage provides enough energy density to compete with other modern energy storers it also prevents all the safety issues primarily caused by high pressure storage. There are 2 main routs for solid state hydrogen storage, both use host materials: adsorption and chemisorption based. Last one can be considered as the most promising of two since it possesses adjustable sorption-desorption parameters. In this case the best host material is magnesium due to a maximal capacity of 7.6 wt%. Nevertheless, there are negative sides of magnesium sorption performance such as poor kinetics and high desorption temperature. To improve these parameters nano crystallization and usually transition metal-based additives with addition of carbon nanotubes (CNTs) (as a catalysts) can be used. During my MSc, a basic investigation of ball milled magnesium hydride catalyzed with FeTi was performed. Intriguing results gave a push for profound analysis of a given material with application of extreme processing techniques such as High-pressure Torsion (HPT).

Research work in the current semester:

Additional MgH_2/FeTi samples were prepared and processed to conduct profound phase evolution during heating measurements (results were included into the listed below article).

Thermodynamics of HPT MgH_2 samples catalysed by FeTi with and without CNTs was investigated by calorimetry measurements. Phase transformation and approximate phase fraction data was obtained after heating up to 800 °C which induces full dehydrogenation of the hydride sample.

Position sensitive XRD measurement was performed on several rotation MgH_2/FeTi HPT disc. Resulted patterns provided microstructural information for given sample with strong deformation degree correlation which can be evaluated by convolutional multiple whole profile fitting.

Publications:

Révész, Á.; Paramonov, R.; Spassov, T.; and Gajdics, M. Microstructure and hydrogen storage performance of ball-milled MgH_2 catalyzed by Fe-Ti. *Energies* 2023, 16(3), 1061. https://doi.org/10.3390/en16031061

Studies in the current semester:

Subject code	Subject name	Lecturer	Credits	Require ments	Class per week	Grades
FIZ/1/024	Lattice defects I.	Gubicza Jenő	6	exam	2	5 (Excellent)
FIZ/1/038E	Diffraction methods in Materials Science I.	Gubicza Jenő	6	exam	2	5 (Excellent)