Structure and Dynamics for Hydrogen Storage in Hydrogen-Rich Alloys

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Introduction

Background:

Titanium-iron (**TiFe**) is known for its hydrogen storage capabilities at room temperature, high volumetric capacities (**0.096 kg_{H2}/L**). However, it is prone to **oxide** layer formation upon exposure to air, requiring energy-intensive activation processes.

Challenges and Solutions:

1. Elemental Doping: Incorporating different transition elements as **dopants** can potentially replace **Fe** and **Ti** in the crystal **lattice structure**, enhancing lattice **size** and creating new diffusion pathways.

2. Mechanical Processing: Post-mechanical processing offers further solutions to these challenges.

3. Research Gap: Limited studies exist showing **correlative**, **quantitative** understanding between **crystallographic** structures and H_2 **sorption** properties for TiFe metal-alloy systems doped with elements: **Nb**, **Ta**, **V** and in combinations.

Research Objectives and Methodologies

This project aims to address this gap by synthesizing TiFe samples with varied **Nb**/**Ta**/**V** stoichiometries using synthesis techniques: vacuum arc-melting (**VAM**) and mechano-chemical synthesis (for ex: **ball-milling**).

Utilizing state-of-art **characterization** techniques: Synchrotron powder X-ray diffraction (**S-PXRD**), X-ray Absorption Spectroscopy (**XAS**), Extended X-Ray Absorption Fine Structures (**EXAFS**) analysis to locate dopant **position** in TiFe crystal structure and understand its related effects on H_2 uptake/storage properties.

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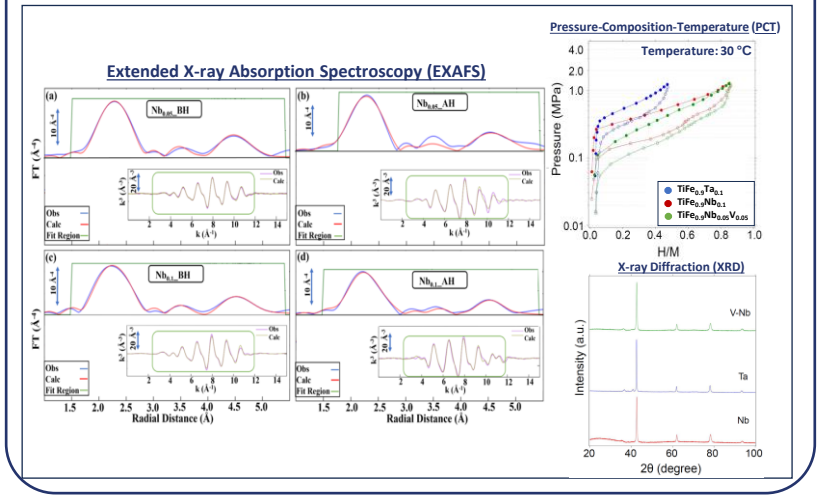
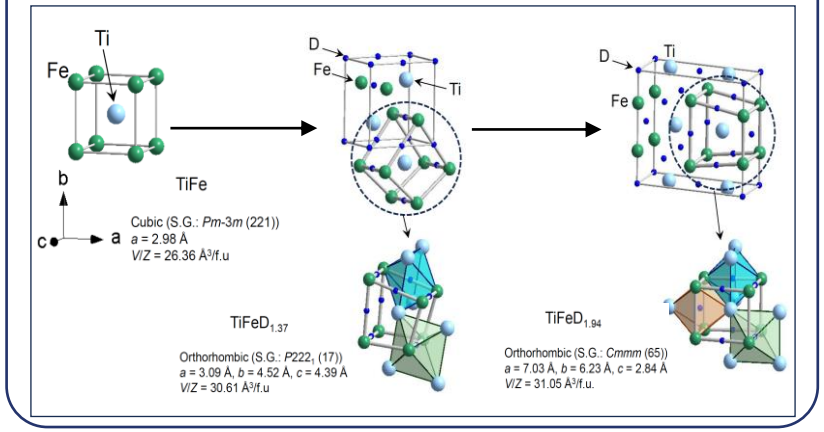
Characterization Techniques to Understand Fundamental Properties



Hydrogen Storage Methodologies



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Related projects: ***Hydrogen som Energibærer, Equinor***

Short Bio

- ***Masters (Ms) in Materials Physics from Norwegian University of Science and Technology (NTNU), Norway.***
- ***Currently pursuing PhD in Physics and Mathematics, from University of Stavanger (UiS).***

Estimated progress of the PhD project:

Just started ...	< 50 %	> 50 %	Almost done ☺

Publications/Conferences

- *Deciphering Atomic Structure and Hydrogen Sorption Kinetics and Uptake of TiFe-Nb doped Metal-Alloys utilizing Combined Techniques: Synchroton PXRD and EXAFS Techniques. **Banerjee, A.**, Deledda, S. and Zavorotynska, O. (2023) 'Research Exchange Program (REP)', Oral Talk. Tokyo: Shibaura Institute of Technology (SiT), 22nd Aug–3rd Nov, 2023.*
- *Deciphering Atomic Structure and Hydrogen Sorption Kinetics and Uptake of TiFe-Nb doped Metal-Alloys utilizing Combined Techniques: Synchroton PXRD and EXAFS Techniques. **Banerjee, A.**, Deledda, S. and Zavorotynska, O. (2023) 'Gordon Research Conference (GRC) - Hydrogen Metal System', Poster Presentation, Les Diablerets, 25th June-30th June, 2023.*
- *Sharma, A., Foppen, J. W., **Banerjee, A.**, Sawssen, S., Bachhar, N., Peddis, D., & Bandyopadhyay, S. (2021). Magnetic Nanoparticles to Unique DNA Tracers: Effect of Functionalization on Physico-chemical Properties. Nanoscale Research Letters, 16(1), 1-16. [24]. https://doi.org/10.1186/s11671-021-03483-5.*

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