Defect Engineering for Solid State Batteries

- Modelling Dislocation Mediated Ion Diffusion in Ceramics

Are you interested in the cutting-edge field of materials science, and looking for an exciting Master's project that could make a real impact on the world? Look no further than our project in defect engineering for solid-state batteries, with an emphasis on understanding dislocation mechanisms in ceramic electrolytes!

Description

As the world shifts towards a more sustainable future, solid-state batteries are emerging as a promising alternative to traditional lithium-ion batteries, offering higher energy density, improved safety, and longer cycle life. However, they are also subject to a range of defects that can impact their performance, such as grain boundaries, dislocations, and vacancies. Dislocations can create regions of localized strain and act as a fast diffusion circus of matter. Their complex behaviour at the atomic scale poses a significant challenge for researchers seeking to optimize their performance and durability. Our Master's project will give you the opportunity to explore these defects in detail, using cutting-edge computational methods to model the behaviour of dislocations - atomic-scale defects that can affect the mechanical properties and ionic conductivity of materials. By exploring the behaviour of dislocations in solid-state batteries, you'll help to uncover the fundamental mechanisms underlying their performance, and pave the way for the development of more efficient and durable battery technologies.



Dislocation-toughened ceramics^[1]

Objective

In this master programme, emphasize is on the exploration of the role of dislocation in determining the mechanical and electrical properties of the ceramic electrolytes used in solid-state batteries. The following aspects should be included:

1) *Literature review*: A comprehensive review of the literature on dislocations in ceramic electrolytes, including the relevant experimental and theoretical studies, to highlight the current state-of-the-art and identify knowledge gaps that the project aims to address.

2) *Model development*: Development of a physical based computational model to simulate the behaviour of dislocations in the ceramic electrolyte materials. This involves the use of dislocation dynamics simulations in combination with finite element modelling. The model will be thoroughly validated and verified against experimental data to improve its accuracy.

3) *Analysing*: Establish fundamental understanding of the mechanics of dislocations in particular ceramics and identify the mechanisms by which dislocations affect the ionic conductivity.

As a part of this program, you'll have access to cutting-edge computational resources and a team of expert mentors who will guide you through every step of your project. You'll gain invaluable experience in materials science research and contribute to the quest for sustainable energy technology. With the potential to publish your findings in high-impact scientific journals and present your research at international conferences, this is an opportunity that could take your career to new heights.

Don't miss out on this exciting opportunity to contribute to the future of energy technology. Apply today for our Master's project in dislocation dynamics modelling in solid-state batteries!

If you're interested in learning more, or require additional information, please feel free to get in touch with us by contacting: Dr. Fengxian Liu (<u>f.liu-3.utwente.nl</u>), or Prof. Inna Gitman (<u>i.m.gitman@utwente.nl</u>)

Reference

[1] Porz L, Klomp A J, Fang X, et al. Dislocation-toughened ceramics[J]. Materials Horizons, 2021, 8(5): 1528-1537.