



PhD Proposal 2017

School: CentraleSupélec	
Laboratory: SPMS	
Team: Functional materials for Energy applications	Head of the team: Gianguido Baldinozzi
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Collaboration with other partner during this PhD:	In China:

Title: Modeling of ion-conducting polycrystals through molecular dynamics

Scientific field: Materials Science

Key words: molecular dynamics, ion conduction

¹ Put here 1, 2 or 3 email personal addresses, separated by commas, of colleagues who will have access to folder of student candidates on the web site. Do not use generic laboratory addresses.

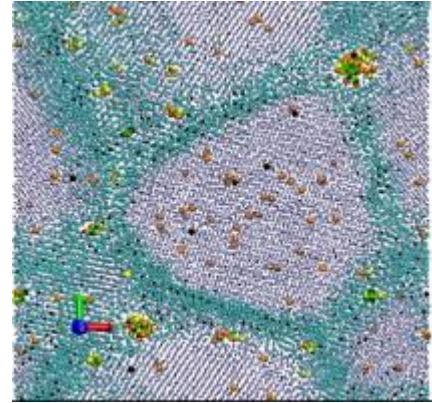
Details for the subject:

Context and objectives:

Solid Oxide Fuel Cells are Solid Oxide Electrolyzers will occupy a strategic place in a near future. Their actual limit lies in their short life, due to fast degradation of components at high temperature. In particular, the polycrystalline nature of the membrane leads to fastened degradation, the grain boundaries being at the origin of cell failure and of additional resistance at low temperature.

The reasons why grain boundaries are more resistive are only partly known, even if the existence of a space charge zone with a depletion of charge carriers is widely accepted.

The objective of this PhD will be to build polycrystalline materials and to test their mechanical and electrical response by molecular dynamics calculations.



Implementation :

The approach is based on the use of analytic potentials to describe the interaction between atoms. Specific potentials will be developed from *ab initio* DFT calculations using a robust potential fitting approach.

Polycrystalline structures will be then created from Voronoï diagrams with a random distribution of grains. A special attention will be paid to the grain boundary zone where atom overlapping might occur by construction. Then, molecular dynamics calculations will be performed that will allow having a clear picture of the influence of GBs on ion conduction properties. Attention will be paid to the visualizing of strain and charges in the grain boundary zone.

The same polycrystal will be then used to evaluate the plasticity at high temperature. This will be compared with available experimental results.

References:

Oxygen diffusion mechanism in the mixed ion-electron conductor $NdBaCo_2O_{5+x}$

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Geneste , **G. Dezanneau**

J. Materials Chemistry, 22, 18744, **2012**

Effects of biaxial strain on bulk 8% yttria-stabilised zirconia ion conduction through molecular dynamics

G. Dezanneau, J. Hermet, B. Dupé

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Int. J. Hydrogen Energy, 37, 8081-8086, **2012**

Oxygen incorporation in acceptor-doped perovskites

E. Bevillon, **G. Dezanneau**, G. Geneste

Physical Review B , 83, Article N° 174101, **2011**