Project report 2020

SIAEROSIM

Simulation of Silica aerogels

MAIN PARTICIPANTS

			
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OVERVIEW *(keep within this page)*

Starting year: 2019 **Current researchers** (permanent/non-permanent): 9 person-month/year

Positioning *(Multiple selection allowed – total 100%)*	**Transportation**	**Energy**	**Eng. for Health**
Materials and structure design		34%	
Surfaces and interfaces		33%	
Simulation and modeling		33%	

Other:

Include partner from ☐ Outside ELyT ☐ Industry

Main funding source(s)
☐ Public project(s) ☐ Industrial ☐ Own resources

IFS CRP/LyC project? ☐ Yes ☒ No

For main projects: Agency / year / name of project *(up to 3, past projects in gray)*

- International Society for Advanced Drawing Breakthrough project, 2021-2023, COMCOM
- ANR-JST project, 2016-2019, COMICA
- PHC, 2014-2016, Sakura

Estimated annual budget: 0

Highlights & Outstanding achievements *(3-5 bullet points)*

- Creation of Silica aerogel with OH group on its surface using reactive interatomic potential
- Definition of the strategy to simulate heat transfer.

Illustration *(5x5 cm² max)*

PROJECT DESCRIPTION

Background

Silica aerogel are highly porous materials, more than 90% porosity. The characteristic size of the pores is few nanometers. Due to these characteristics, silica aerogels have a thermal conductivity which is lower than the thermal conductivity of air. Even if the production cost is expensive, they are used in each case the insulating volume and mass has to be minimized (transportation, housing…). Silica aerogels are good candidate to help reducing energy consumption.

However, material aging is an issue since in building the material properties should not vary during several tens of years. Silica aerogels present two drawbacks: low mechanical properties and an increase of the thermal conductivity with time. This is due to the high porosity of the material:

- The higher the porosity, the lower the thermal conductivity at the expense of the mechanical properties.
- The nanostructure of silica aerogel increases the specific area of the material and surface reactivity. Silica reacts with water vapor which leads to the thermal conductivity increase.

Mechanical and thermal properties of silica aerogel depend on the atomic structure of the material. Their predictions thus require the atomic scale simulation of silica aerogels. It is done using Molecular Dynamics simulations. During his PhD (2013-2016), W. Gonçalves choose and studied an interatomic potential to predict mechanical properties of pure silica aerogels [1,2]. Within this framework, Morthomas et al. [3] proposed a strategy to predict the thermal properties of pure silica aerogel. W. Kassem as part of a post doc (AURA region funding, Pack Ambition project) studies the adequate interatomic potentials for realistic simulation considering the surface chemistry of silica aerogels.

Key scientific question

The goal of the project is to use another kind of interatomic potential that account of the surface chemical reactivity in order to:

- Predict the thermal conductivity of realistic silica aerogel considering surface chemistry. This study may allow optimizing the production process.
- Study the influence of water vapor on the modification of the nano structuration of the aerogel and then the influence on the thermal conductivity and mechanical properties.

Research method

The research method is based on Molecular dynamics simulation of a silica aerogel system on which OH group have been added on the surface.

The use of reactive interatomic potential leads to a drastic reduction of the number of atoms compared to previous simulations. So only silica nanowires are considered.

The simulation strategy consist first to create the silica nanowires and then to add OH group on it.

Then the news nanowires are submitted to mechanical and heat transfer test to predict the influence of the OH group on their mechanical and thermal properties.

Research students involved *(gray color for previous years)*

Bachelor student:

- Aikaterina Kiourtzidou, from Aristotle University, Thessalonique, Greece. Intern at MATEIS from October 2019 to April 2020. Aikaterina Kiuortzidou presented a poster during the ElyT Workshop 2020.

Visits and stays *(gray color for previous years)*

FR to JP (date, duration):

- T. Tokumasu
  - Feb. 20 , 2020
  - March 9-10, 2020
  - Nov. 18-20, 2020

COMMUNICATIONS AND VALORIZATION

Journal publications *(gray color for previous years)*

	Authors	Title	Journal	Vol.	pp. / ID	Year	DOI
1							
2							

Conferences *(gray color for previous years)*

	Authors	Title	Conference	Date	City	Country	DOI *(if applicable)*
1	Takashi Tokumasu, Patrice Chantrenne and Aikaterini Kiourtzidou	Prediction of thermal and mechanical properties of Silica Aerogel using atomic scale simulations	LyonSE&N – ELyT – IARI Workshop 2020 – 11th annual workshop	February 17th -19th, 2020	Vogüé, Ardèche	France	
2							

Patents *(gray color for previous years)*

	Inventors	Title	PCT #	Year
1				
2				

Others *(gray color for previous years)*

	People	Event	Description	Date
1				
2				