

Master internship offer

(from February/March 2019 – 5 to 6 months)

Development of a kinetic model for the SiO_xN_y deposit by CVD and numerical simulation of the process

LGC – ENSIACET (France)

In an ongoing collaboration, CIRIMAT, LGC and an industrial partner developed proprietary, high throughput CVD processes able to uniformly coat the inner surface of complex substrates by amorphous SiO₂ films. They were processed from tetraethyl orthosilicate, TEOS and O₂ below 580 °C, i.e. the upper limit of the mechanical conformity of the substrates. The aim was to form coatings protecting the substrate from aqueous corrosion.

Despite the excellent barrier properties, unacceptable, important concentration of leached Si ions from the films was revealed. These partial failures demonstrate the need to study new coatings with regard to the imposed specifications, and to optimize their properties.

In this frame, new works are planned to deposit innovative SiO_xN_y coatings from a mixture composed of TEOS/O₂/ozone and a N containing species. The deposition route is completely new and the window of deposition conditions will have to be defined by combining an experimental study on lab-scale CVD reactors and numerical works of process simulation.

The Master internship only concerns the simulation part. Numerical codes of process simulation already exist into LGC for the SiO₂ deposit in two CVD reactor configurations. The master student will first have to learn and master these codes. A new kinetic model will then have to be developed for the SiO_xN_y deposit, using the available bibliographic data and the experimental results obtained by the PhD student involved in this project. This model will be implemented in the codes and validated by comparison with the experimental data. Optimization routes of the process could be finally proposed using the validated model, to reach the target coating thickness and composition.

This offer concerns students preparing a Master 2 (or equivalent) in Chemical Engineering, with a first experience in process simulation using CFD codes (Comsol, Fluent, ...). A good level of English is required, as an ability to teamwork.

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