**Title of the thesis:** Multi-scale modelling of the mechanical and thermal properties of cementitious phases.

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**Extended abstract:**

The development of computational methods to describe and predict the mechanical properties of cement-based materials is of obvious practical importance. The accuracy of the prediction of mechanical or, from a more general point of view, physical properties depend largely on the knowledge of the intrinsic properties of the various constitutive phases. Up to now, these properties have been solely obtained by experimental procedures. The tremendous increase of computational capabilities has largely favoured the development of numerical modellings based on a realistic and multi-scale description of these kinds of materials.

Since several years, the future Ph-D supervisors have been involved in the development of such numerical tools from the micro- to the macro-level (see for instance [Bernard et al., 2008; Kamali-Bernard et al., 2009; Comby-Peyrot et al., 2009; Bernard et al., 2010; [Bernard et al., 2012]; [Bernard et al., 2014]). The so-called MuMOCC (Multi-scale Modeling Of Computational Concrete) platform has thus been developed. The intent is to assist the material developer by providing a rational approach to material development and concurrently assist the structural designer by providing an integrated analysis tool that incorporates fundamental material behaviour.

It is now clear that any realistic attempt to accomplish such an objective should be based on appropriate nano-structure / performance relationships: the properties depend much on the chemico-physical properties of the interatomic bonds. That is why more recently the simulation methodology used in the framework of the MuMOCC platform has been extended to the atomic scale: the atoms are pictured as spheres; their electronic nature is taken into account implicitly with some parameters such as their charge and their radius. The interactions between atoms are also considered: ionic (Van der Waals and Coulomb forces) and chemical forces. This is the topic of the PhD thesis of Jia Fu (CSC program 2012-2016) [Fu et al., 2015a; Fu et al., 2015b; Fu et al., 2015c; Fu et al., 2015d] where several numerical methods have been developed and investigated to this purpose (Density Functional Theory, Atomic Finite Element Method and Molecular Dynamics).

The objective of this new proposal is to pursue these last works.

Two different objectives are proposed in function of the curriculum vitae and the scientific background of the successfully candidate:

1. It is first proposed to study in more details the C-S-H phase (Calcium Silicate Hydrates, the main hydrates of the cementitious materials, responsible for their strength). The crystal structure of C-S-H in cement paste has not been fully resolved yet and there is still ongoing debate over its nanostructure, that is why several models proposed in the international
scientific literature will be considered in order to construct a Representative Volume Element of this phase and to determine, by means of Molecular Dynamics simulations, its main mechanical properties. That includes also the study of the creep behavior since the C-S-H phase is the main hydrate of the Hardened Cement Paste which exhibits such a time-dependent behavior.

The second part of this first topic work will focus on the up-scaling of the results obtained at the atomic level in order to connect this modelling to continuum models by using relevant input from this level and carrying forward the critical information to represent the continuum with the intrinsic nano-scale features incorporated into the model.

2. The second objective is dedicated to the physical origins of thermal properties of cement paste. Despite the increasing interest in multi-scale cementitious materials, very few studies concern the determination of the thermal properties at the nanoscale and their connection to the macroscale properties. In this study it is thus proposed to combine various modelling tools to achieve such a goal: probably Density Functional Theory and MuMoCC platform developed by the supervisors of the PHD thesis, particularly in the field of mass transport. The numerical developments will then applied to the modelling of the thermal properties of bio-based cementitious materials in the framework of the sustainable development.

The up-coming thesis is mainly based on simulation and numerical developments. However the work will require validation with experimental procedures (for instance micro-traction tests, nano-indentation tests or measure of thermal conductivity).

References


Fu J., Bernard F., Kamali-Bernard S., Nano-scale modeling and elastic properties of a typical CSH (I) structure based on DFT and Molecular Dynamics Methods, Rencontres Universitaires de Génie Civil, May 2015.