Computational multiphysics 3D homogenization framework for the design of fast-curing dental composites

Gerry Agbobada*, **Pierre-Olivier Bouchard***, **Yannick Tillier***

* CEMEF Centre de Mise En Forme des Matériaux
MINES ParisTech, PSL Research University
CNRS UMR 7635 CS10 207, 06904 Sophia Antipolis Cedex
e-mail: gerry.agbobada@mines-paristech.fr, web page: http://www.cemef.mines-paristech.fr/

ABSTRACT

Having a precise material state after the polymerisation reaction is crucial to run fatigue simulations for methacrylate resin-based composites such as those used in dentistry (Bis-GMA, UDMA, TEDGMA. . .). The shrinkage that occurs during the polymerisation leads to residual stress, and sometimes to debonding at the interface with dental tissue.

These composites share a relatively high volumetric filler fraction and a random microstructure with **strongly heterogeneous properties, even within the resin** since the filler are silanized to promote adhesion with resin. Hence, the Computational Homogenization method has to be used to model the quick polymerisation reaction of such composites and its consequences on the mechanical behaviour [1].

Within a first-order Computational Homogenization framework, **temperature, strain and degree of conversion of the resin are computed at the micro-scale** in order to model the fast, constrained reaction. An in-house adaptive meshing tool allows us to work on any microstructure using a **conforming, unstructured mesh** of P1+/P1 elements [2]. After a discussion on the choice and the **implementation of boundary conditions** on Representative Volume Element (RVE) with unstructured meshes [3], different models of resin-filler interactions are compared to see their influence on the homogenized behaviour. The relevant size of the RVE is chosen with percolation possibilities in mind.

Resulting simulations are compared to macroscopic scale and microscopic scale experimental tests to choose the best **interactions model at the resin-filler interface**. With these results, failure and fatigue models will be added in order to predict lifetime of these materials.

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References

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