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Multiscale Modeling of Thermal Shock: From Microstructure to Failure
I. Özdemir, W.A.M. Brekelmans and M.G.D. Geers
Eindhoven University of Technology, Department of Mechanical Engineering

Introduction
Refractories are used to build structures subjected to high temperatures, such as the metallurgical furnace linings in metal, glass and ceramic manufacturing industries, Fig.1. Depending upon the application, refractories must resist chemical attack, withstand molten metal erosion, thermal shock and other adverse conditions.

These structures are highly sensitive to damage due to thermal shock, which is basically cracking, stemming from rapid temperature changes. At the micro level, expansion/contraction differences due to temperature gradients and inherent anisotropy in the thermal expansion coefficient results in microcracking along the grain boundaries, which in turn leads to macroscopic cracking, Fig.2.

Objective
The long term objective of this study is to develop a multiscale mathematical model to investigate thermal shock failure. The micromechanics based model will allow to investigate the effect of microstructural variables (e.g. grain size and shape) on the thermomechanical damage and to optimize the microstructure for certain applications. The project consists in the integration of recently developed numerical techniques, where additional features related to the stress build-up through time-dependent thermal gradients has to be added.

Modeling
The thermal and mechanical problem, and possibly their coupling will be treated within the framework of computational homogenization. The basic idea is the derivation of the macroscopic material response from the underlying microstructure by solving a boundary value problem at the micro level. To this end, at first a computational homogenization procedure is developed for the heat conduction problem.

The macroscopic temperature \( \theta_M \), and the temperature gradient \( \nabla_M \theta_M \) are applied as external loading for the microstructural domain. Upon the solution of the microboundary value problem, the macroscopic heat flux \( \mathbf{q}_M \) is obtained by a proper averaging relation and the macroscopic conductivity \( K_M \) by a condensation procedure, Fig.3. The problem is assumed to be steady-state at the micro level. Therefore the heat balance equation,

\[
\nabla_m \cdot \mathbf{q}_m = 0
\]  

(1)

holds over the micro domain with Fourier’s law of heat conduction for each microstructural constituent as,

\[
\mathbf{q}_m(\mathbf{x}, \theta_m) = K_m(\mathbf{x}, \theta_m) \cdot \nabla_m \theta_m
\]  

(2)

Essentially, the heterogeneity and nonlinearity of the conductivity at the micro level is accounted for and transferred to the macro level.

Future Work
The thermal homogenization will be combined with the mechanical homogenization\cite{1} including cohesive elements to investigate the thermal shock failure.

References:
\cite{1} KOZNETSOVA ET AL: An approach to micro-macro modeling of heterogeneous materials (Comp. Mech., 27, 37-48, 2001)