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Silica-filled rubber: Effective-medium modeling

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Introduction
Constitutive modeling of nanocomposites to predict their mechanical performance is the focus of a large number of studies, due to the practical importance e.g. for car tires. In this study, we examine rubber filled with nanometer-sized silica particles.

Important aspects in tire applications are adhesion (grip), internal losses, and wear. Addition of hard nanofillers into the rubber network leads to the Payne and Mullins effects. Nanofillers also drastically affect the tear-behavior of the sample, particularly the crack shape (see Fig. 1) and the amount of absorbed energy.

![Fig. 1. Different tear-behavior of unfilled and filled rubber.](unfilled Rubber localization avoid stress filled rubber)

To describe the behavior of the silica-filled rubber, the system is considered on different, but tightly inter-related scales (see Fig. 2):
- **Macroscopic level**;
- **Microscopic level**.

Goal
The goal of this project is to formulate a macroscopic description of the silica-filled rubber (constitutive equation), taking into account the effects of the filler-particles, e.g. the glassy layers around and the glassy bridges between them.

Current status
The macroscopic formulation, according to Fig. 2, for large deformations and nonisothermal conditions has been achieved (Eulerian and Lagrangian), by using the non-equilibrium thermodynamics formalism GENERIC [1,2].

References

Macroscopic level
From a macroscopic perspective, silica-filled rubber can be described by two elements in parallel:
- **Spring** – to describe the rubbery network; this rubber modulus enters into the thermodynamic potential (elastic strain energy);
- **Spring and dashpot** in series (Maxwell element) – to describe the effect of glassy bridges; this high effective modulus does not enter into the thermodynamic potential, because it is a transient effect only.

![Nodes in FEM](unfilled rubber filled rubber)

Relative arrangement of particles
- Single particle is surrounded by glassy layer
- Pair-correlation function
- Representative Volume Element (RVE)

Microscopic level
On the microscopic level, silica-filled rubber can be described in two different ways (see Fig. 2):
- For each RVE, there is an effective relaxation time, which depends on the local stress, temperature, and particle arrangement.
- **Pair-correlation function**. The particle arrangement is accounted for in terms of the pair-correlation function. Knowing for every node the pair-correlation function, one can build from the behavior of a particle-pair the response of the entire RVE.