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MODELLING OF STRUCTURE EVOLUTION OF FILLED ELASTOMERS UNDER UNIAXIAL ELONGATION

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ABSTRACT

Interaction of rubber matrix and fillers provides the basis for modern materials with remarkable properties, as high stiffness, high tensile strength and at the same time large extension ratios until fracture, which resulting in specimen lengths that exceed the initial size of a material several times [1]. As it is well known the fillers, in particular carbon black, consist of fractal aggregates built by the coalescence of single particles (shape of particles close to spherical) [2]. These aggregates form agglomerates with different sizes, which finally result in filler clusters or filler networks depending on the filler concentration.
The evolution of the filler network structure in elastomers during elongation is investigated on the basis of computer modelling. The filler network is represented by spherical particles of different sizes, which are randomly filling a prismatic volume. Interpenetrations of particles during modelling of filling and subsequent stretching are forbidden. The material is assumed to be incompressible.
We intend to provide a technique that describes realistically the isotropic initial structure of injection moulded composites with low computational requirements and hardly predefined particle size distribution and distance between them, which can be subsequently used for the determination of the structural changes during deformation of the composite. Aggregates or agglomerates of a filler network are assumed as separate spherical particles.
The basic model of the composite material is represented by a rectangular prism with a square base, as shown in Fig. 1, with an initial height of volume – H_0 and the base sizes - L_0.
The algorithm of adding the i-th particle to an existent set is based on the percolation model when particles are placed in a free space of matrix. The particles are not allowed to touch each other, but their surfaces have to remain in a minimal distance $d_{min.}$

Two cases of filler volume fractions are examined: dense and loose filled. For this purpose the minimal distance between the surfaces of spheres during construction was set equal to d_{min} =10nm or d_{min}=100nm, respectively.

Deformation is carried out stepwise by stretching the filled material along the *z*-axis (Fig. 1). Invariability of volume because of the assumed incompressibility is taken into account with the help of the elongations along the three axes: $\lambda_x \lambda_y \lambda_z = 1$. In a

material with a high filler fraction originally close particles can depart from each other over a distance that some times exceeds the change of the length of the material. This is the result of particles that collide with each other during stretching of the material. Thus essential remixing of fillers occurs. Thus, these links should withstand huge deformations and to be extremely strong.

During deformation the coordination number in a material with high filling decreases with increasing elongation. The analysis of the pore size has shown that during stretching of a material essential heterogeneities are formed - areas where the density of particles becomes very high and at the same time spaces free of fillers are created.

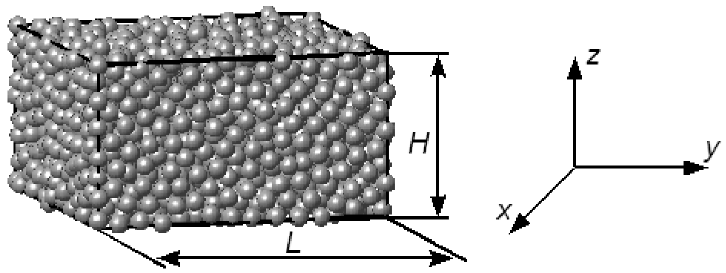

Fig. 1. Model of the carbon-particle filled elastomer, initial structure.

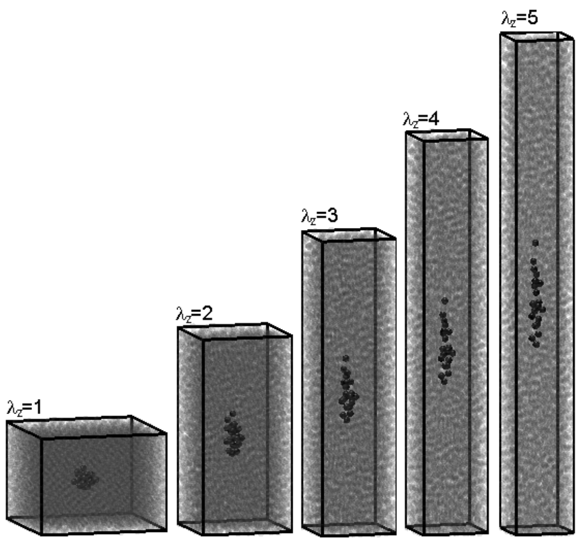

Fig. 2. Structural changes of the material during stretching.

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