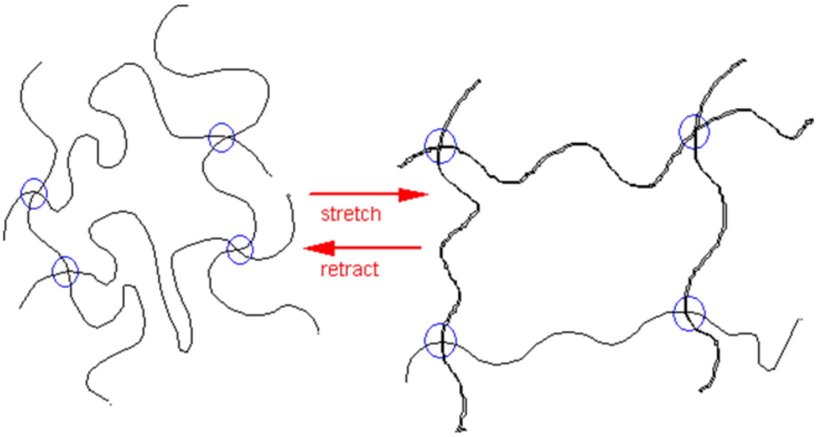
Masters project

Computational Design of Structural Materials

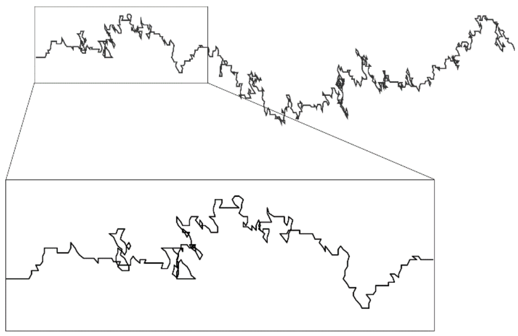
Numerical modelling of elastomer chain microphysics

Background



Elastic polymers (elastomers) are a group of materials that have rubber-like properties, i.e., can undergo extensive reversible deformations; their use is widespread in current industrial applications and in new research areas [1].

These polymers have no crosslinking in the liquid state, so their chains can change their position due to Brownian motion. Therefore, the polymer chains form a loose three-dimensional network[2]. After vulcanisation polymer chains form cross-links that allow the material to retract after deformation.



Under tension, the elastomer chains stretch out along the applied force direction and return to their original state after that force is lifted. Such structure can be numerically described by scaling laws or fractal dimension[3]: segments of polymer chains can be represented as random walks, which on a larger scale build up into polymer chains that obey the same statistical laws. The effect of chain and cross-link distribution on the mechanical behaviour of rubber is an urgent problem in the field of polymer mechanics.

Project goal and objectives

This project is a part of a larger PhD project "Multiscale analysis of polymer composites," where mass-fractal theory is used to describe the geometry of reinforced polymer composites' mesostructure numerically. The goal of this project is to apply the fractals or scaling laws to create a model of the underlying microstructure of the polymer matrix. The macroscale behaviour of elastomers can be analysed through numerical modelling of microscale deformation mechanisms using a physics-based model of coiled cross-linked polymer chains.

Thus, the objectives are:

1) Investigate available literature on polymer chain scaling law (or fractal) description.
2) Adapt an existing fractal model of a polymer chain to describe the mechanical behaviour of the polymer (such as S-SBR) undergoing finite deformations on the microscale.

The expected outcome of this project is a geometrical model suitable for FEA.

Contact: Dr. ir. I. Gitman: i.m.gitman@utwente.nl or E. (Lisa) Karaseva: e.karaseva@utwente.nl

[1] Jacob D. Davidson, N.C. Goulbourne, A nonaffine network model for elastomers undergoing finite deformations, Journal of the Mechanics and Physics of Solids, V. 61 (8), 2013
[2] P.J. Flory, *Principles of Polymer Chemistry*, New York 1953
[3] P.G. de Gennes, Scaling Concepts in Polymer Physics, Cornell University Press, Ithaca, NY, 1970