

# Multi-scale Studies of Elastomers (*in a tire tread*)

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A tire tread is a nanocomposite in a particular shape, which has to ensure good grip for safety without neglecting other performances such as wear or rolling resistance, the latter being actually directly related to the fuel consumption of the vehicles. It is well known that the material processing has a great impact on the properties of treads and more quantitative relationships are still under investigation. One possibility is to achieve improvements by considering the process/product as a whole, but another possible approach is to design an optimized structure for one or several properties by coupling theory / simulation / structure analysis, and then develop the process which would allow reaching the desired target. The presentation will focus on the step “design of an optimized structure”.

Several properties of the tire tread materials are mainly governed by the polymer dynamics. As the dynamic properties of a polymer melt involve a large interval of relaxation times, a multi-scale approach is necessary for its study. From atomistic simulations (Molecular Dynamics done with Materials Studio from Accelrys), we can only obtain information about the high frequency / high temperature polymers behavior. However, from the obtained atomistic configurations, we are also able to develop for different polymers the so-called “realistic mesoscopic interaction potentials” (usable in DPD or more general CG simulations) with an inverse iterative Boltzmann method [1], in particular deriving a method for the NPT ensemble [2,3]. These mesoscopic potentials allow to obtain good static properties such as the squared end-to-end vector  $\langle R^2 \rangle$  or the rubbery plateau modulus  $G_p$ , which cannot be reached with classical MD simulations. Work is still in progress to also obtain the polymer dynamics from chemically realistic DPD simulations. Optimizing the polymer network topology and the effect of confinement on polymer chains is also under investigation through chemically realistic DPD simulations, similarly as what has been done in references 4 and 5 in order to understand respectively the non-affinity during swelling and the modification of the entanglement density near a wall.

[1] Lahmar F. et al., *Onset of entanglements revisited. Topological analysis*, *Macromolecules*, 2009, 42, pp 7474 – 7484.

[2] Maurel G., Schnell B., Goujon F., Couty M. and Malfreyt P., *Multiscale modeling approach toward the prediction of viscoelastic properties of polymers*, *JCTC*, 2012, 8, pp 4570 – 4579.

[3] Maurel G., Goujon F., Schnell B. and Malfreyt P., *Prediction of structural and thermomechanical properties of polymers from multiscale simulations*, *RSC Advances*, 2015, 5, pp 14065 – 14073.

[4] Saalwächter K. et al., *Swelling heterogeneities in end-linked model networks : a combined proton multiple-quantum NMR and computer simulation study*, *Macromolecules*, 2004, 37, pp 8556 – 8568.

[5] Vladkov M. and Barrat J.-L., *Local dynamics and primitive path analysis for a model polymer near a surface*, *Macromolecules*, 2007, pp 3797 – 3804.