

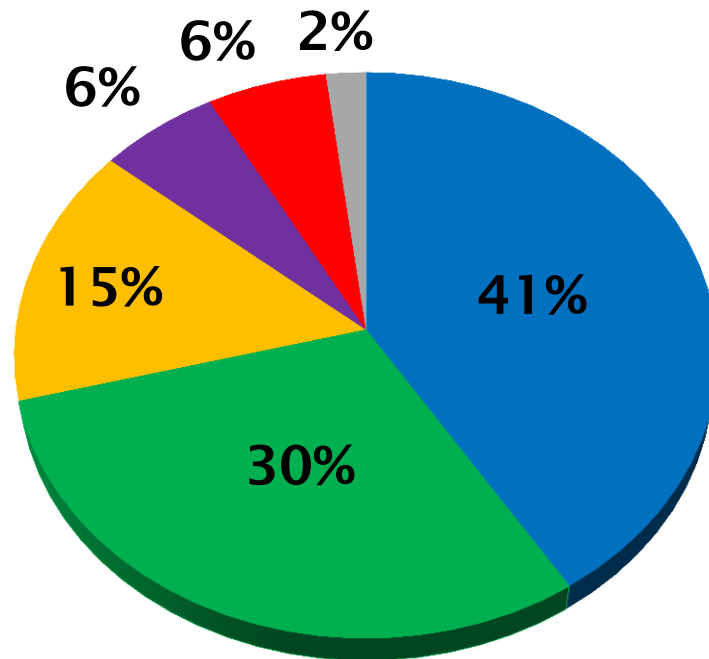
Coarse-Grained Molecular Dynamics Simulations of Polymer-Solid Interfaces in Nanocomposites

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Tyre Components and Composition



- Rubber
- Fillers
- Reinforcing Materials
- Plasticizers
- Chemicals for Vulcanisation
- Anti-Ageing Agents and Others

Rolling Resistance



Driving Conditions

Wet Grip



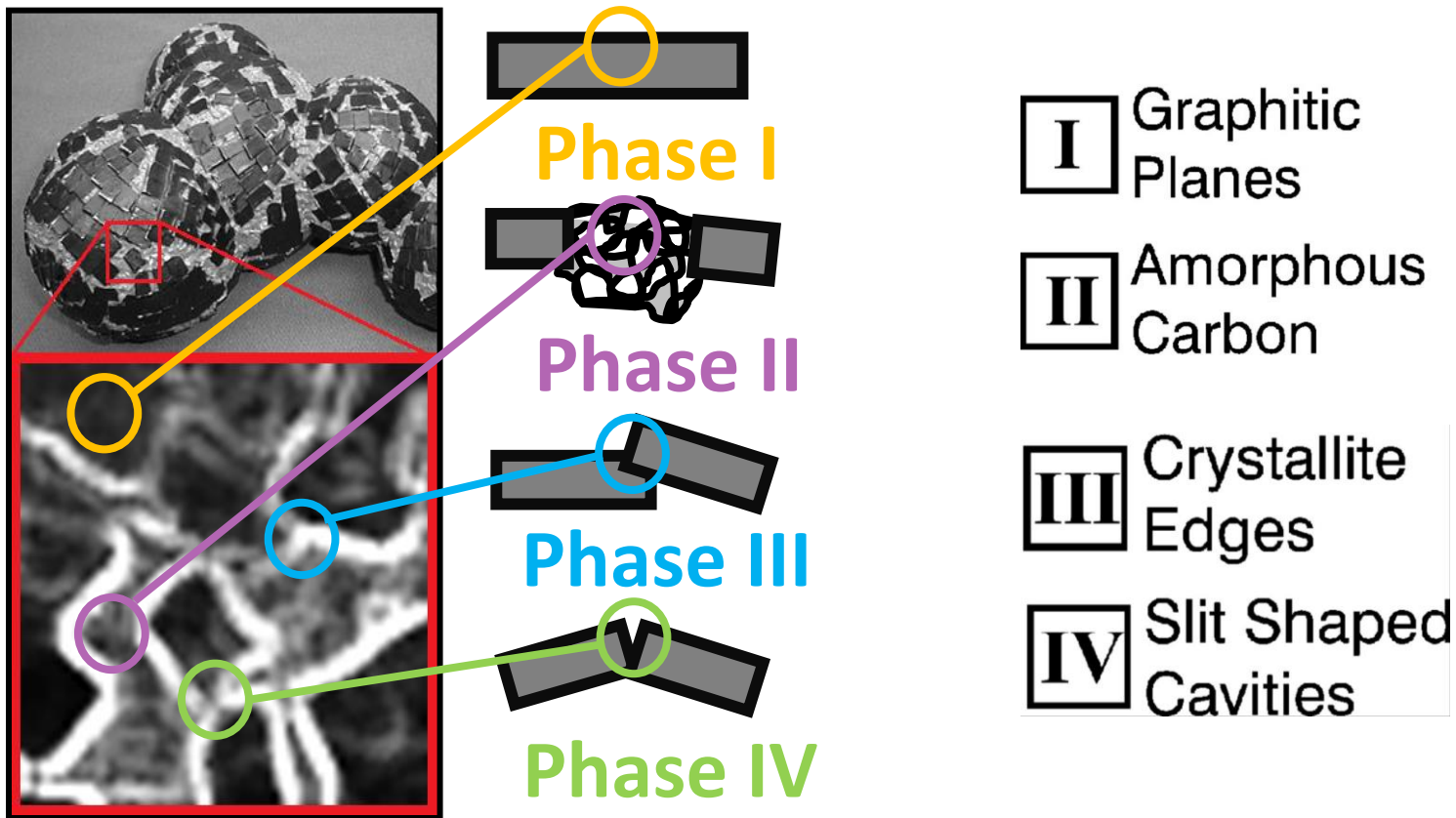
Wear Resistance





Carbon-Black Surface

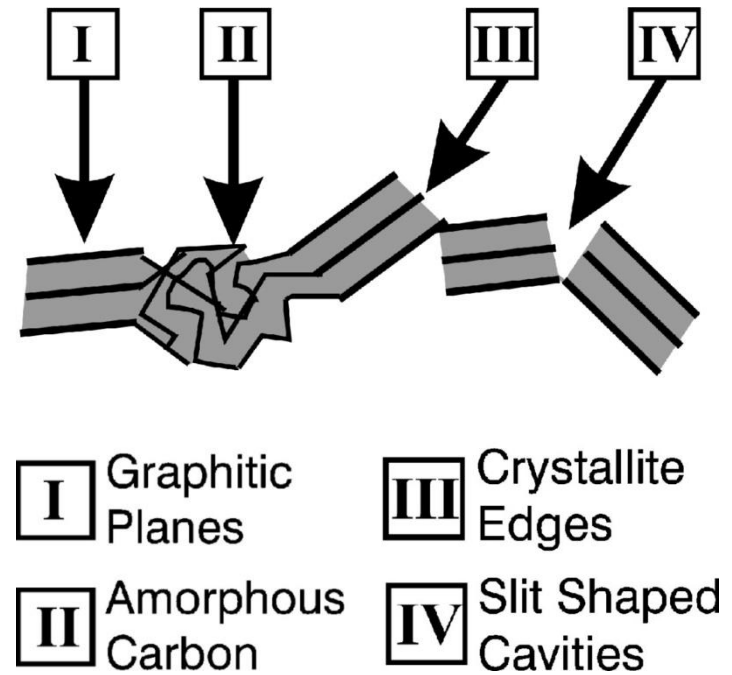
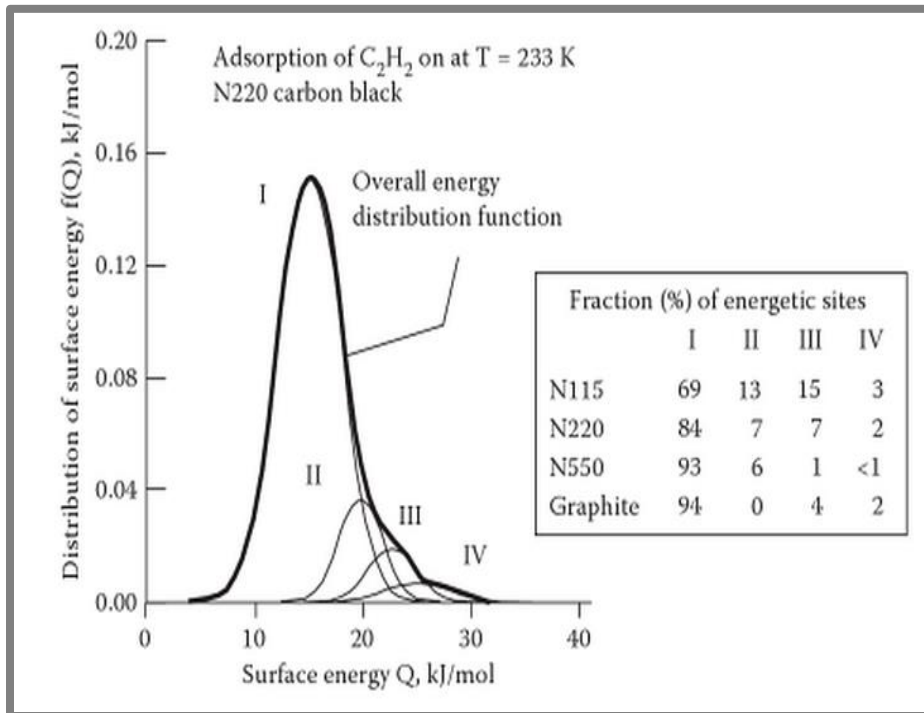
Modelling the effects of surface roughness on the interactions between a heterogeneous surface with a polymer melt.





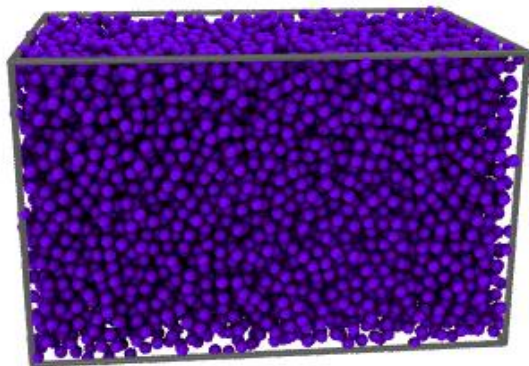
Carbon-Black Surface

Each phase on the surface has been experimentally shown to have an associated adsorption energy. The site energy distribution function $f(Q)$ was determined from the gas adsorption isotherms of ethene.





Polyisoprene Melt

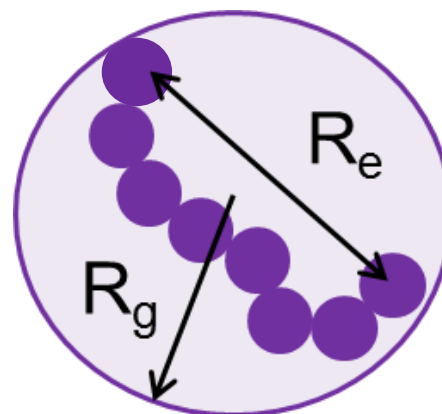
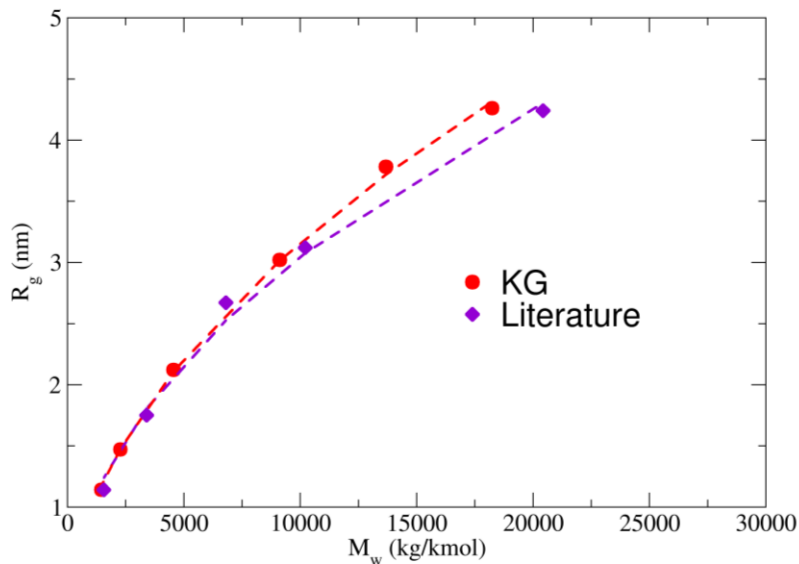


$$R_e^2/M_c \text{ (\AA}^2\text{mol/g)}$$

Experimental* 0.679

Simulation 0.658

*Svaneborg, C., et al. 2016 *arXiv preprint arXiv:1606.05008*



$$R_g = 0.027N^{0.51}$$

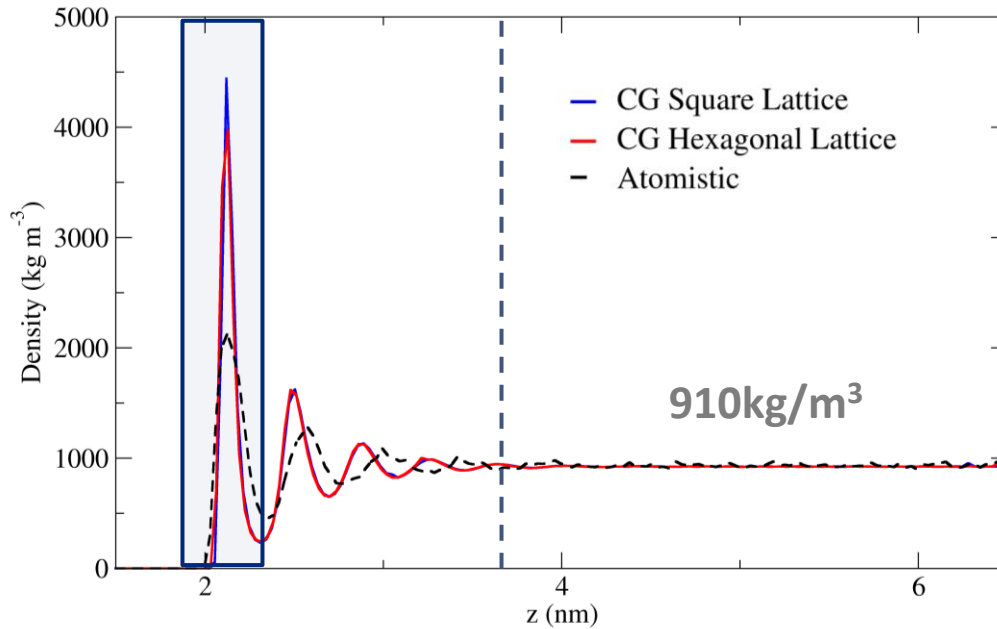
$$R_g = 0.035N^{0.48}$$

Pandey, Y. N. et al. 2014 *J. Chem. Phys.* 140(5), 054908



Interfacial Structural Properties

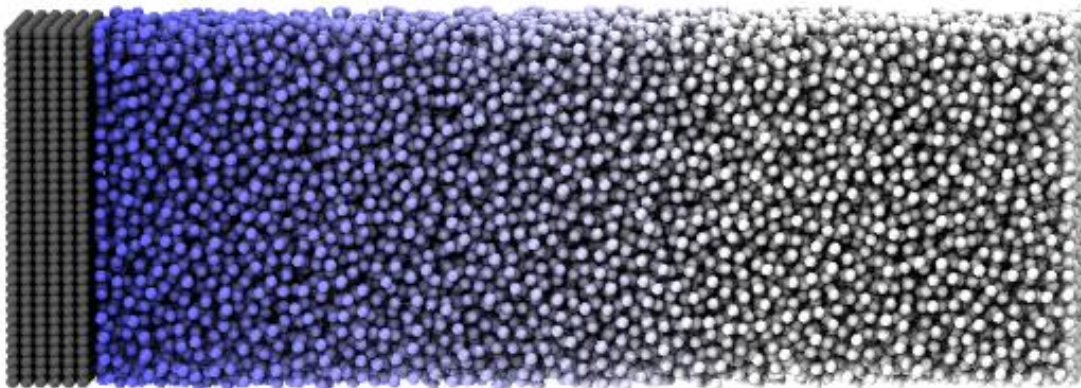
Adsorbed Region



Approaching the bulk the density profile is asymptotic with an uniform local mass density corresponding to that of the polymer melt.

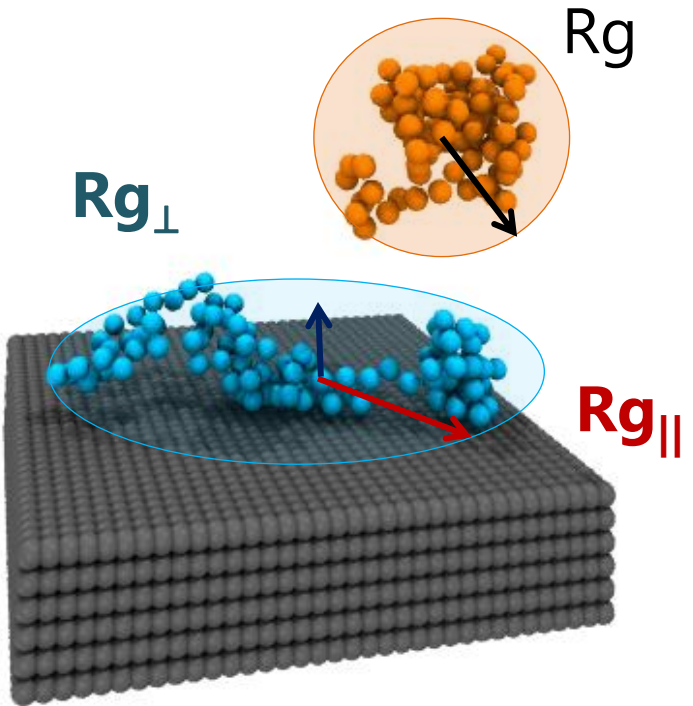
Interfacial Layer

Bulk

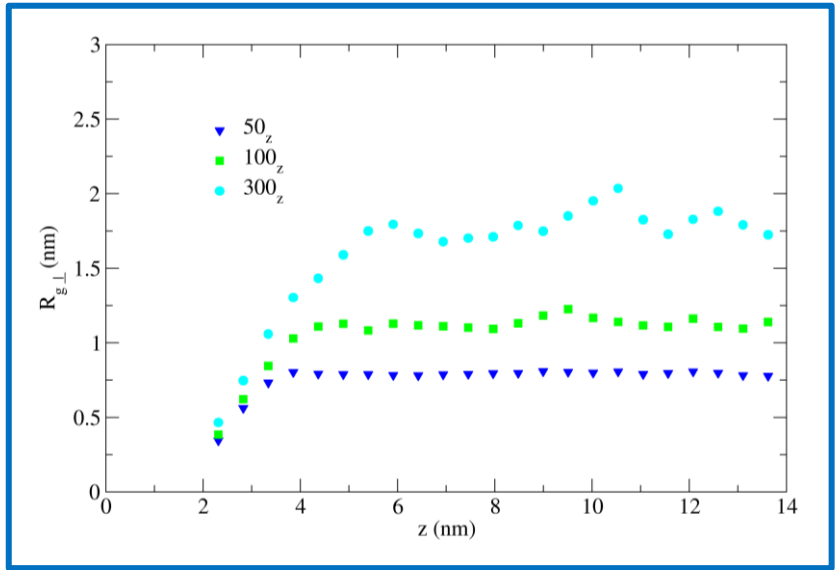
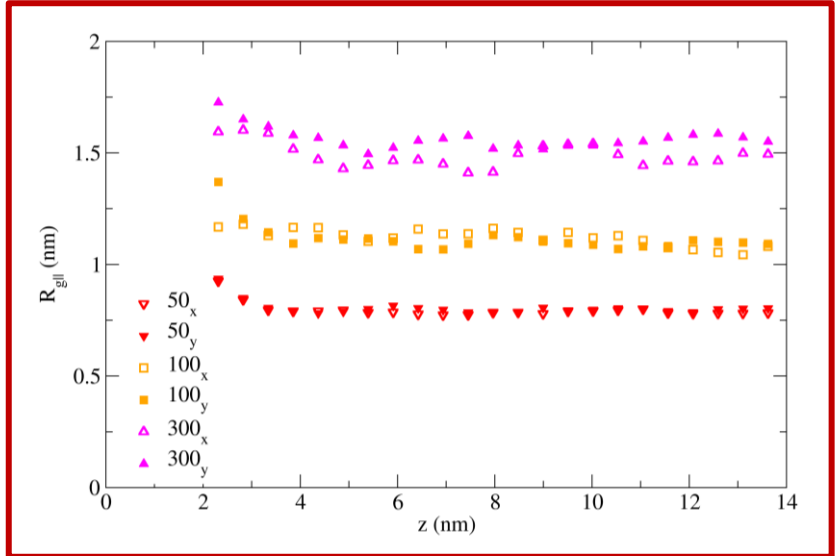




Adsorbed Chain Conformation



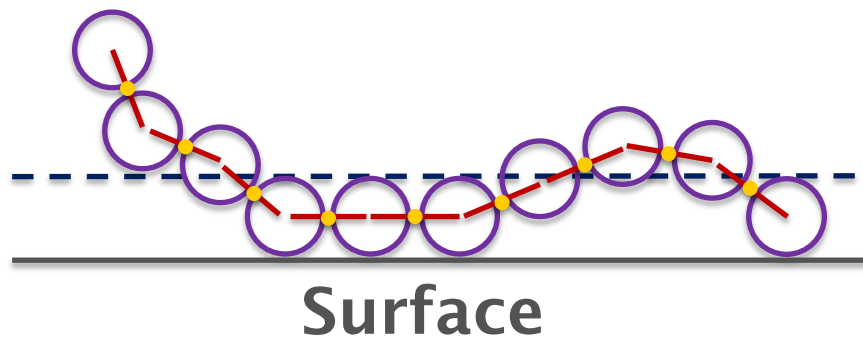
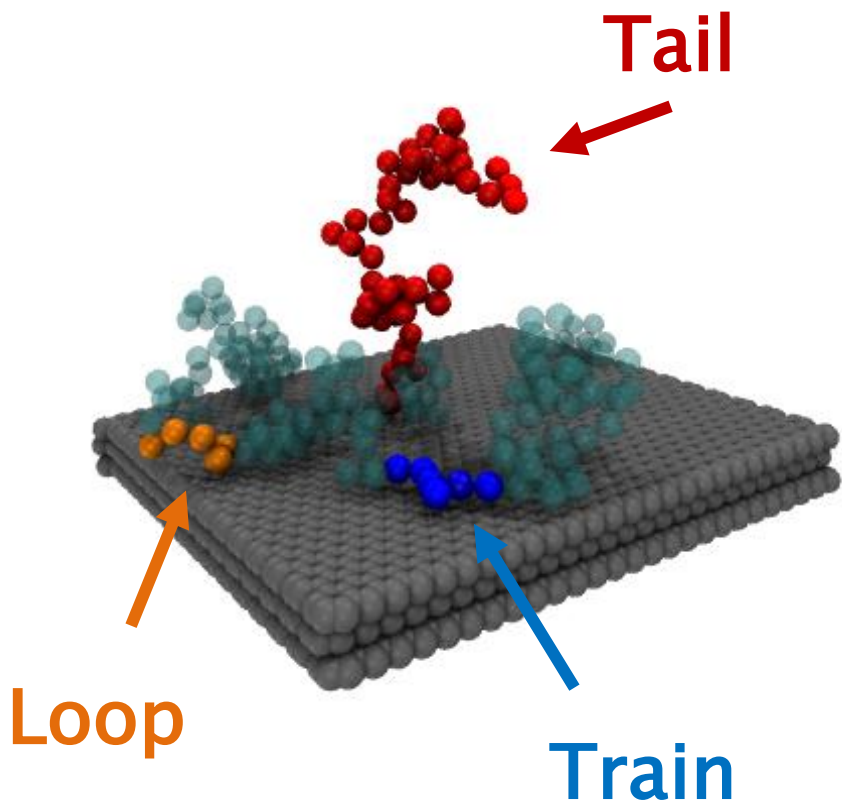
The adsorbed chains assume a “pancake structure”: flatted in the direction parallel to the wall and compressed in the perpendicular direction.





Adsorbed Chain Conformation

Many properties of polymer nanocomposites are determined by the conformation that the polymer chains adopt in the immediate vicinity of the surface.



N. Tails=1 Length=2

N. Trains=2 Length=4 and 1

N. Loops=1 Length=2

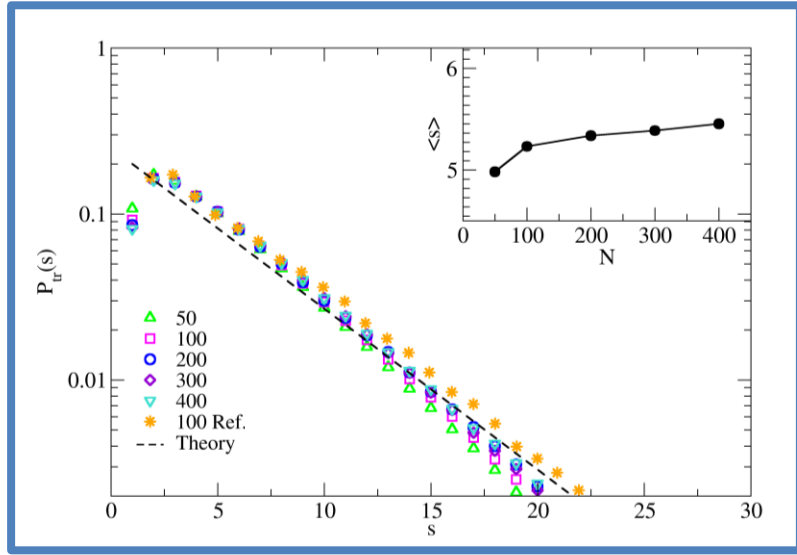
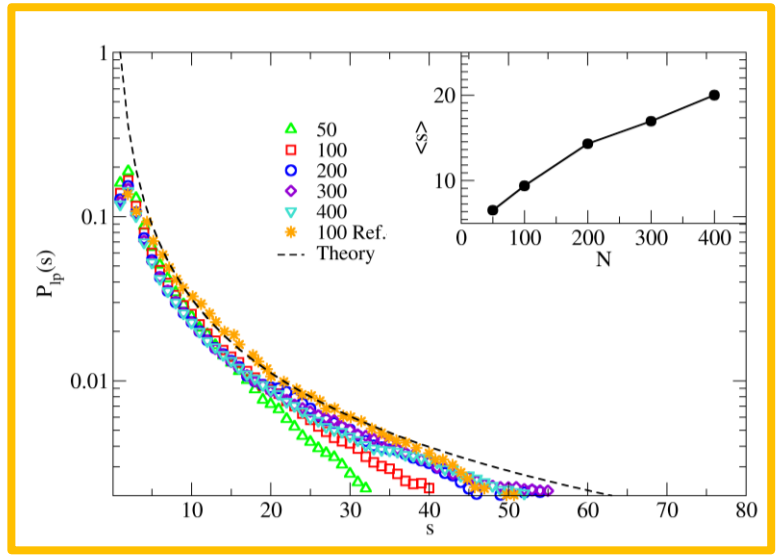
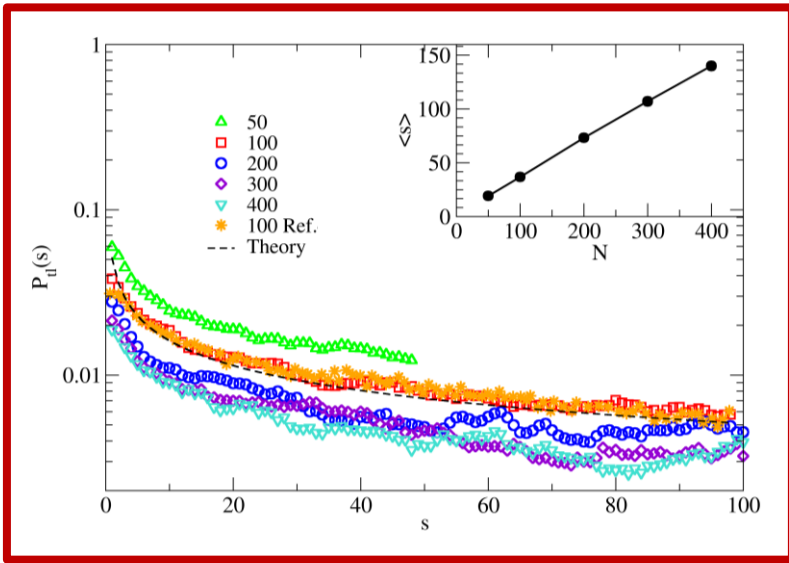
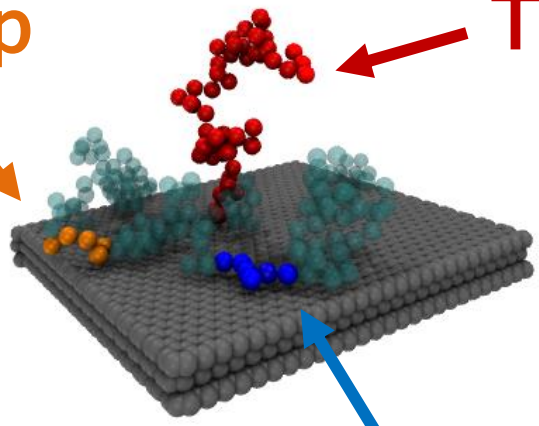


Adsorbed Chain Conformation

Loop

Tail

Train

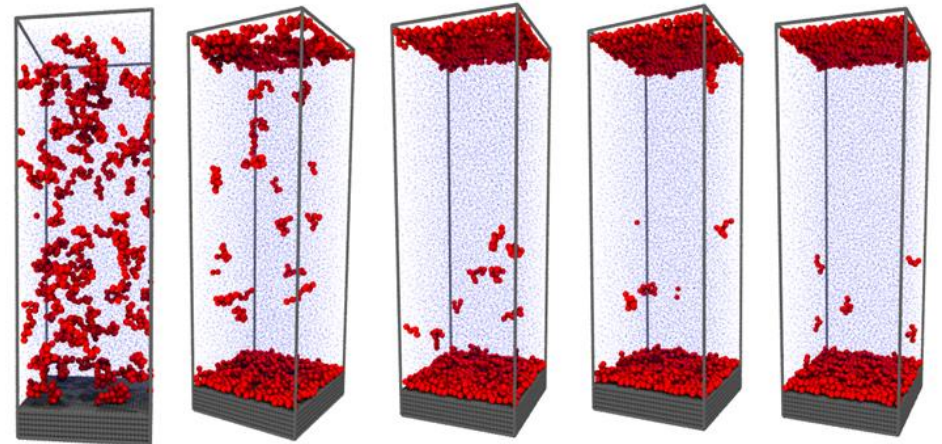
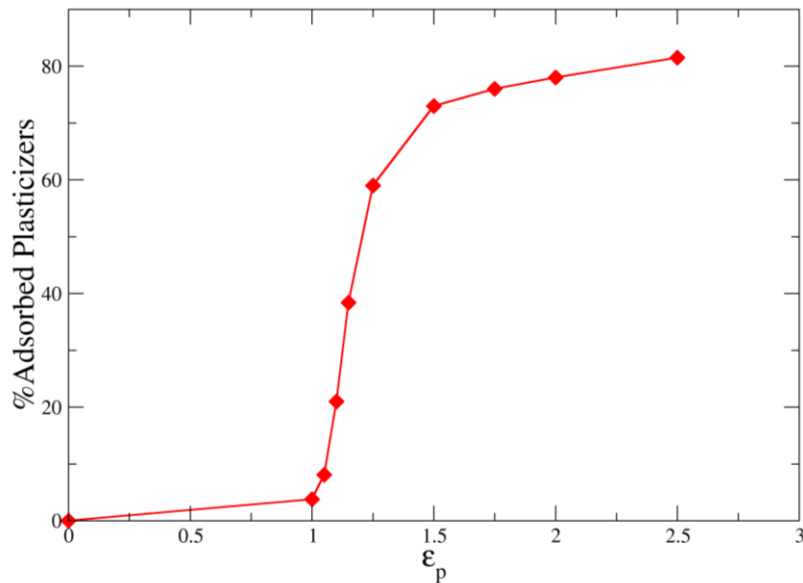




Plasticizers

A method to modify the glass transition temperature of polymers is to add a small amount (~5phr) of plasticizers.

- Polyisoprene
- Plasticizers



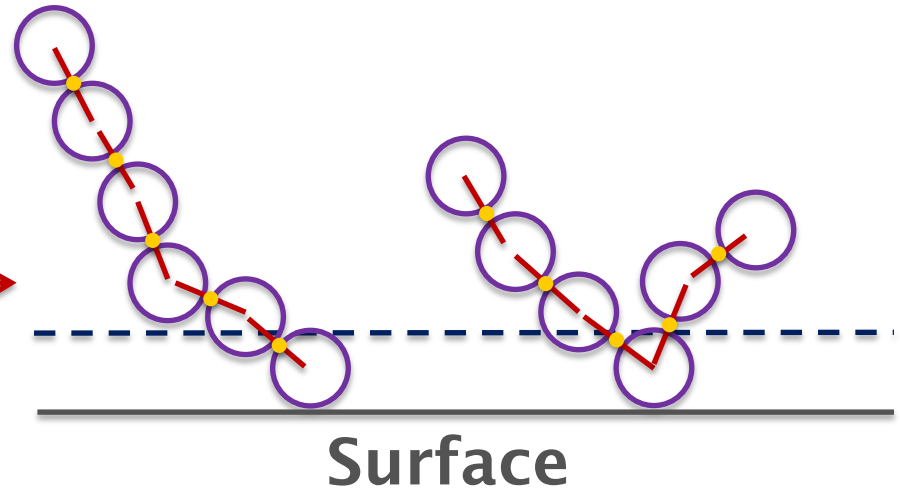
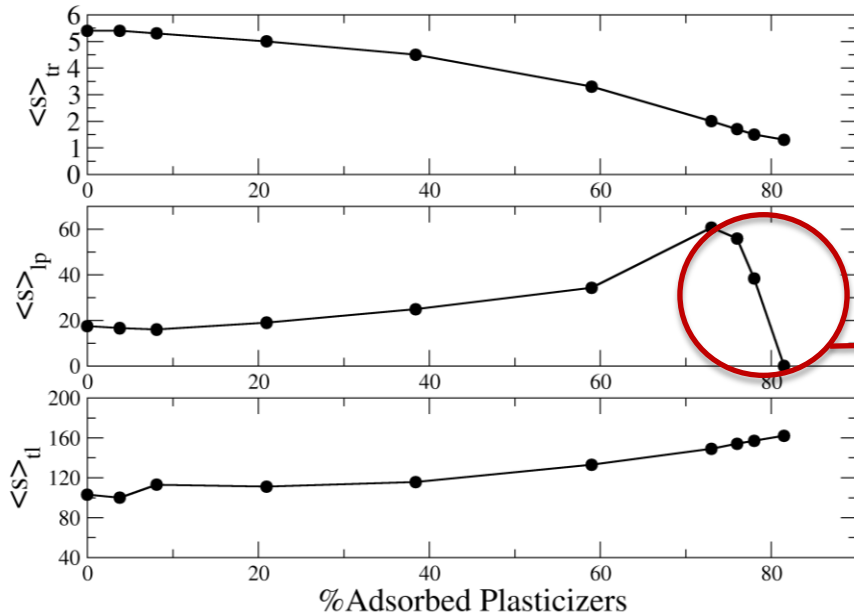
1 1.25 1.5 1.75 2

$$\epsilon_p = \frac{\epsilon_{PL-S}}{\epsilon_{PI-S}}$$



Plasticizers

Trains Loops and Tails



As the percentage of plasticizers adsorbed on the surface increases, the average length of trains decreases indicating that the polymer chains desorb from the surface.



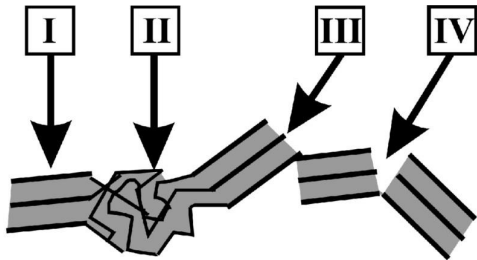
Conclusions

- ✓ A Coarse Grained model for polyisoprene on graphite was developed and validated.
- ✓ The attractive force at the interface polymer/surface influences the structural features, i.e. density profile, radius of gyration, chain conformation.
- ✓ The presence of the plasticizers influences the structure of the polymer in the vicinity of the surface.



Future Work

- Adsorption of polymer chains in contact with rough surface (realistic carbon-black surface).



I Graphitic
Planes

II Amorphous
Carbon

III Crystallite
Edges

IV Slit Shaped
Cavities

- The change in chain conformation and polymer adhesion to the surface under shear.



Acknowledgments



The University of Manchester



Multiscale Modeling Group



Thank you for the attention!

