

Static and dynamic properties of polycarbonate blends adsorbed on a nickel surface

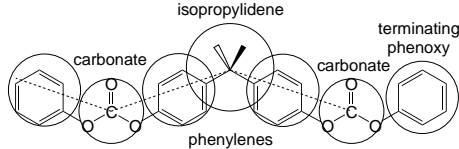
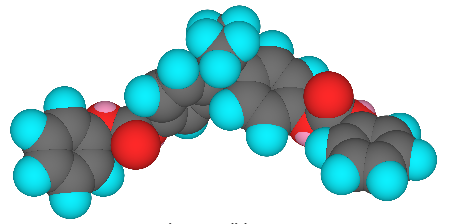
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Motivation

Why polycarbonates?

- High impact strength, ductility, high glass transition and melting temperatures, good mechanical and optical properties
- Ideal material for compact discs, automotive components, and ophthalmic applications [1]
- Attractive test system for the coarse-graining techniques [2]

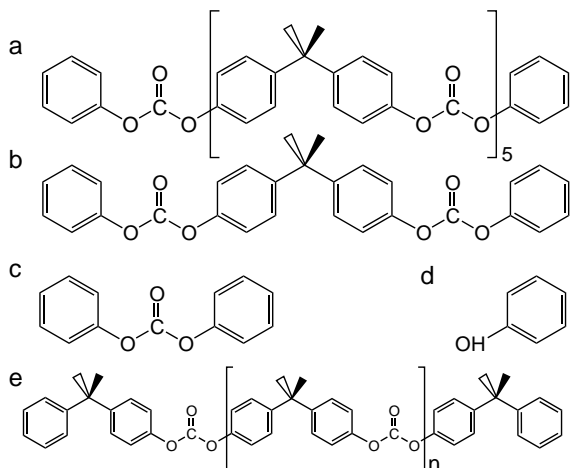


Chemical structure and coarse-graining scheme of a bisphenol-A-polycarbonate (BPA-PC) molecule. Only one repeat unit is shown.

Simulation details

Studied systems

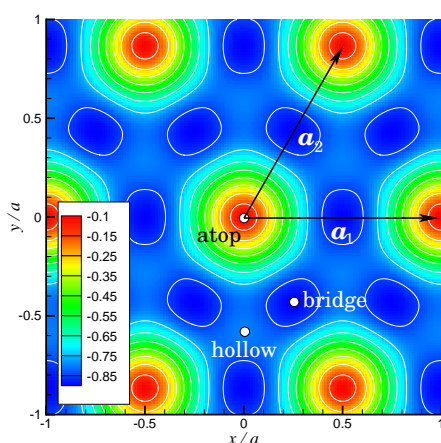
The host polymer is the phenol terminated BPA-PC of $N_1 = 20$ repeat units. The second component (5% in weight) is BPA-PC of $N_2 = 5$ repeat units, one repeat unit, diphenyl carbonate (DPC), or phenol.



Chemical structures of the studied systems

Interactions

Ab initio calculations [4, 3] suggest that the internal beads have a weak interaction with the surface but phenylene ends are strongly attracted to it.



Contour plot of the chain end - nickel surface interaction potential. Units are in eV, $1eV \sim 20kT$ where $T = 570$ K

A coarse-grained model is used to describe the BPA-PC molecules. Each repeat unit is represented by four beads. The parameters of the interaction are obtained from the MC simulation of a single atomistic chain in vacuum [2].

Simulation details

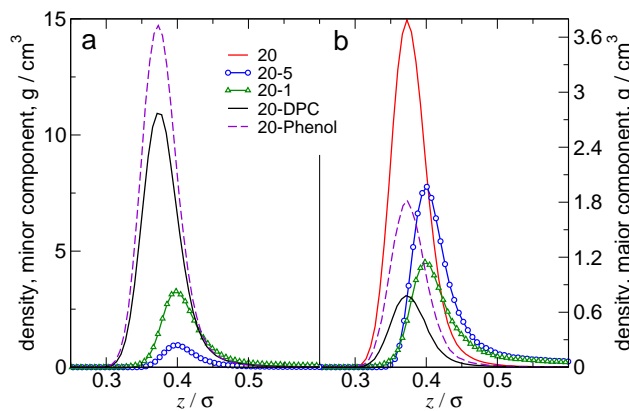
We use NVT ensemble with Langevin thermostat which is switched off in the shear direction. The shear rate is

$$s = 2v_w / L_z \tau_r \approx 10, \quad (1)$$

where τ_r is the Rouse characteristic relaxation time.

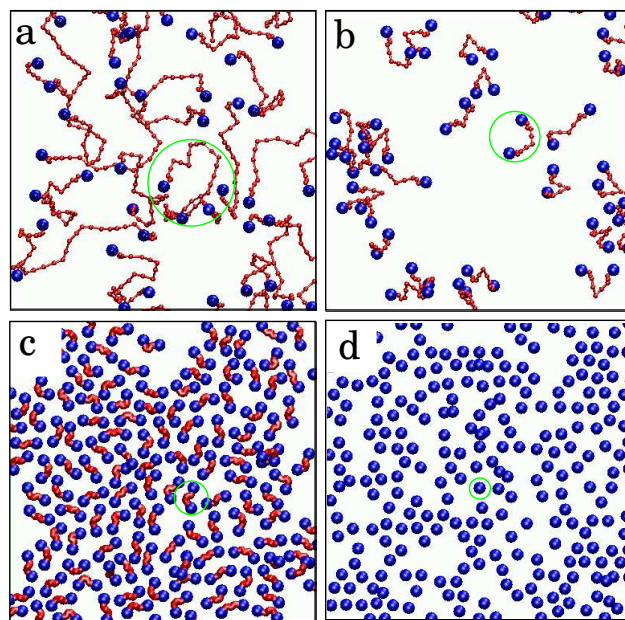
Results

Static case



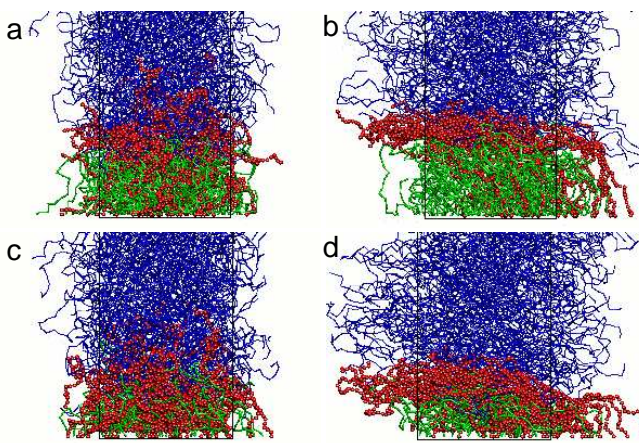
Chain end density profiles for different mixtures.

Diphenyl carbonate provides the most efficient screening of the interaction between the melt and the surface.



Snapshots of the bidispersed melts: (a) 20 : 5 repeat units; (b) 20 : 1; (c) 20 : diphenyl carbonate; (d) 20 : phenol. Only the molecules of the minor component next to one of the walls are shown. The green circle (shown only as an eye-guide) depicts the excluded surface area per a molecule adsorbed on the surface.

Sheared blends



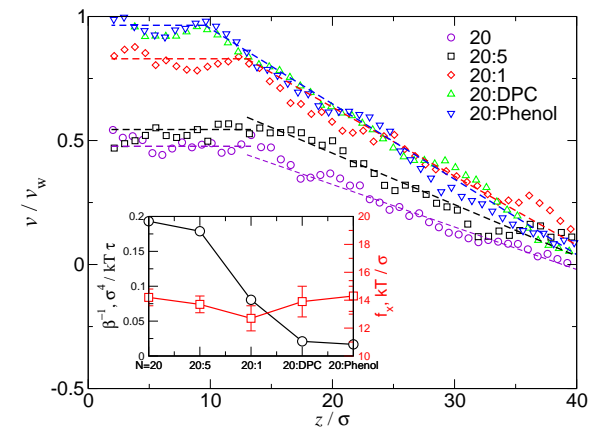
Snapshots of the mixtures: 20:5 without (a) and with (b) shear, 20:phenol without (c) and with (d) shear. Green: chains which adsorb both ends; red: only one end (red); blue: no ends

- The decrease in the number of the adsorbed chain ends of the major component results in thinning of the adsorbed layer.
- Under shear the one-end attached chains disentangle from the melt.

Acknowledgments

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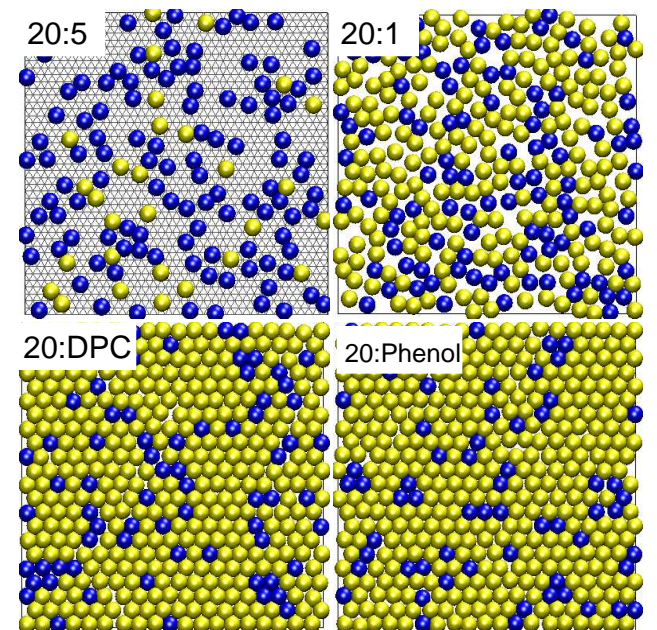
Velocity profiles



Normalized velocity profiles. Inset: the friction force and the friction coefficient.

$$f = \beta(v_w - v_s) = \eta \frac{dv}{dz}. \quad (2)$$

The friction coefficient β depends on the density of the attached chain ends.



Snapshots of the chain ends adsorbed on the wall. The blue beads are the chain ends of the major component, and the yellow - of the additive.

The adsorbed layer of the 20:5 mixture has a structure of a 2D gas; the packing of the 20:1 mixture is similar to a 2D liquid; for the 20:DPC as well as 20:Phenol mixtures the adsorbed chain ends form a 2D crystal.

Summary

- Attractive interaction of the chain ends with the surface results in an adsorbed layer, made of single- and two-end attached chains. Short chains diffuse from the bulk and occupy the adsorption sites much faster than the long ones.
- The smallest melt coverage is achieved for diphenyl carbonate, due to its high mobility and relatively large excluded volume.
- The slip boundary condition changes to the no-slip when the epitaxial ordering of the adsorbed parts of the chains locks the motion of the surface layer.

References

- [1] J. L. DeRudder, *Handbook of Polycarbonate Science and Technology* (Marcel Dekker, New York, 2000).
- [2] C. F. Abrams, and K. Kremer, *Macromolecules* **36**, 260 (2003).
- [3] L. Delle Site, A. Alavi, and C. F. Abrams, *Phys. Rev. B* **67** (2003).
- [4] L. Delle Site, C. F. Abrams, A. Alavi, and K. Kremer, *Phys. Rev. Lett.* **89** (2002).
- [5] X. Zhou, D. Andrienko, L. Delle Site, and K. Kremer, *EuroPhys. Lett.* **70**, 264 (2005).