Predicting Structure Development in Solvent-Borne Blend Systems

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The active layers of organic solar cells are processed using solution-based casting techniques. The films form via phase separation under evaporative conditions of a polymeric donor and a fullerene-based acceptor. As device performance strongly depends on the phase morphology it is highly desirable to predict how solution-state dynamics depend on material properties and processing conditions.

The current paper presents a continuum model based on the minimization of a free energy functional involving local and non-local contributions. Time-resolved numerical simulations of polymer:fullerene:solvent ternaries are presented treating the interplay between isotropic/bulk-interactions and stratifying effects.[1] Scaling relations are derived using an analytical approach that describes the effect of evaporation on characteristic length scales encountered in demixing phase morphologies.[2] Where appropriate, results obtained through calculation and simulation are benchmarked against experimental findings whilst considering the identification of links between phase behavior and -purity and actual device performance.[3]

In Fig. 1 we show a numerical simulation of structure development in a demixing blend under evaporative conditions (left). The right plot demonstrates excellent agreement between numerical and analytical approaches towards predicting the dominant length during early stages of spinodal decomposition.
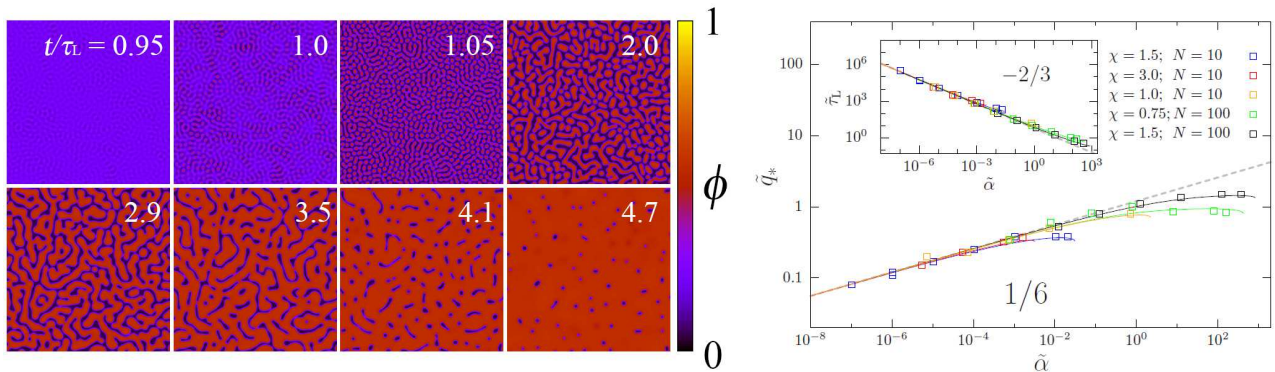

Fig. 1. Left: time-snapshots of a numerical simulation of evaporation-induced structure development in a polymer solution. Right: scaled dominant Fourier mode during spinodal demixing plotted as a function of scaled evaporation rate – points: numerical simulations for various input parameters, lines: linearized theory; inset: scaled time-to-bifurcation versus scaled evaporation rate.

The main conclusion of this work is that in order to capture the full dynamics of solution-processed thin-film blends, classical phase separation theory must be extended to properly incorporate evaporation effects. This work is supported by the Dutch Polymer Institute under grant #734.

References

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