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Molecular Dynamics simulations on stretching of amorphous PPV films

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Abstract – We present a theoretical study of the effect of stretching on the morphology of amorphous PPV films. We use for that classical molecular simulations, with models containing 35000 atoms, and perform statistical analysis of conformation and packing properties.

Poly(p-phenylene vinylene) (PPV) is an important conjugated polymer, with applications on organic light-emitting diodes and in other optoelectronic thin film devices. Usually, amorphous PPV films are obtained via the spin-coating technique followed by a thermal treatment that is useful to improve its performance for applications. Electronic and optical properties of polymer films are closely related to the morphology [1] and indeed, recent experiments [2] have shown that thin PPV-films submitted to mechanical stretching, up to $d/d_0 = 2.0$, show marked differences in the absorption and emission spectra, increasing the emission of polarized light in the direction of stretching.

In this work we have studied the effect of stretching on configurational changes in amorphous PPV films. We performed Classical Molecular Dynamics simulations [3,4] in a model containing 35000 atoms (phenyl-capped chains, formed by 25 monomeric units). We start from a previously optimized configuration that simulates casting at room temperature and pressure. We evaluate the influence of stretching on the resultant morphologies of the film with the aim to estimate the anisotropy in the orientation of the chains. We analyzed the changes in statistical conformational distributions of the chains (linearity and planarity), and the statistical correlation of relative orientation of neighboring phenyl rings, before and after the stretching. Our stretched models are presented, and we discuss the tendency to ordering in the inter-chain packing.

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