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Development of Morphology Landscapes in Polymer Nanofibers during Electro-Spinning

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Spatio-temporal emergence of micro-/nano-porous and gradient structures in electro-spun nanofibers has been investigated theoretically in the context of time-dependent Ginzburg-Landau equation (Model B), alternatively known as Cahn Hilliard equation, coupled with the Fick's law for solvent evaporation across the fiber/air interface. To satisfy the conserved compositional order parameter, numerical simulation was carried out under the quasi-steady state assumption at an extremely small time step. The systems under consideration are solutions of an amorphous polymer and a liquid crystalline polymer. To guide experiments, various temperature - composition phase diagrams of amorphous solution was first established by seeking self-consistent solution. Numerical experiments were conducted in reference to various co-existence regions. The relative rates of solvent evaporation and phase separation have been varied through the choice of spinning temperature and the starting polymer concentration. Depending on the competition between the solvent evaporation rate and phase separation dynamics, various morphological patterns can be witnessed at the fiber cross-section as well as fiber surface such as solid fiber with concentration gradient, hollow fiber with skin-core, phase separated core with smooth skin, and porous fiber morphology through out the skin and the core. The micro-porous fiber surface has been reported for the electro-spinning of polystyrene into the humid environment, but the present calculation reveals that the humidity of not a necessary criterion; a similar structure can develop under appropriate dry-spinning conditions. In support of the present prediction, Liu and Kumar reported the porous skin morphology in electro-spinning of PMMA nanofibers from methylene chloride solutions. A similar study has been extended to a liquid crystalline polymer solution by adding Maier-Saupe free energy pertaining to orientational order parameter and Flory free energy for chain rigidity. The emerged LCP nanofiber morphologies have been discussed in relation to the LCP/solvent phase diagram. Supported by NSF-DMR and NASA.