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Growth modeling and mechanical study of anisotropy of polymer spherulite aggregates by FFT method

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In the present paper, the cellular automaton method is developed to simulate the spherulite pattern formation, where the nucleation is modelled using the concept of random local nucleation time. Based on the kinetics parameters of nucleation and crystal growth rate from experiment results, the spherulitic microstructures under isothermal crystallization are generated, providing the crystallite orientation at each point. Furthermore, considering that the semicrystalline polymers are constructed by lemallea with various local rotations which consist of amorphous phase and crystallites, fast Fourier transform iterative computation algorithm is empolyed study the elastic anisotropy at the mesoscopic scale. The statistical convergence analysis, RVE size analysis are presented, as well as the invariants analysis, from which we determined the RVE size and obtained the anisotropy of elastic tensor. We believe that such approach can provide the elastic information of the semicrystalline polymers with high efficiency, and it is interesting to reveal the R_0-orthotropic behavior of the spherulitic morphology, which is special anisotropic material presenting isotropic Young's modulus.