Effect of Interchange Reactions on the Non-equilibrium Molecular Weight Distribution of Poly(ethylene terephthalate)

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Condensation polymers may undergo interchange reactions during polymerization and processing. Interchange reactions minimize molecular weight fluctuations between polymers and lead molecular weight distribution to the most probable one.

In this study we examine the variation of the non-equilibrium molecular weight distribution of poly(ethylene terephthalate)(PET) with interchange reaction by a Monte Carlo simulation. Chains are packed into square lattice, and a periodic boundary condition is imposed. Two types of motion are allowed in this simulation: the motions based on pseudokinetic motion proposed by Mansfield and reptation. End attacks, backbites and bondflips are allowed, which are analogous to intermolecular alcoholysis, intramolecular alcoholysis and transesterification respectively. If the neighboring site of chain end is unoccupied, the reptation is allowed. It is assumed that no polycondensation occurs in the system.

The results show that number average molecular weight is constant while weight average molecular weight decreases as the number of interchange per segment increases. The molecular weight distribution changes to the most probable one as the interchange reaction progresses. PET samples of non-equilibrium molecular weight distribution are obtained by solution blending of two different average molecular weight PET's. Interchange reactions are carried out through heat treatment. The simulated molecular weight distribution will be compared with the molecular weight distribution determined by gel permeation chromatography.