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缠结高分子熔体非线性拉伸流变中的“缠结-堆积”转变

摘要

管道模型（Tube model）通过将多链缠结的相互作用简化为单链图像，实现了对聚合物材料力学行为的定量描述，并为从聚合物加工到生命科学等领域的应用奠定了基础。然而，在强拉伸流场中，该理论表现出系统性的失效。本文通过对缠结聚合物的分子动力学模拟，揭示了链间构型中存在一种由应变诱导的、从缠结态向堆积态（Packed state）的转变。在原始链（Primitive chain）拉伸达到饱和后，对流解缠结和链取向作用促使体系重新组织为由取向链段构成的二维堆积构型。这种转变从根本上改变了非线性拉伸流中应力的来源，从而解释了管道模型在上述条件下的失效，并实现了对大拉伸应变下力学响应的定量预测。这项研究结果清晰地阐明了链间集体重组是如何主导非线性拉伸行为的。

关键词

高分子物理，软物质凝聚态，复杂流体物理，分子动力学模拟

Abstract

The tube model, which reduces the interaction of many-chain entanglement to a single-chain picture, has enabled quantitative descriptions of the mechanical behaviors of polymeric materials and underpins applications from polymer processing to life sciences. In strong extensional flows, however, this theory systematically fails. Herein, through molecular dynamics simulations of entangled polymers, we reveal a strain-induced crossover from the entangled state to a packed state in the inter-chain configuration. Following the saturation of primitive chain stretch, convective disentanglement and chain alignment reorganize the system into a packed configuration of aligned segments. This crossover fundamentally alters the origin of the stress in nonlinear extensional flows, which explains the breakdown of the tube model under such conditions, and leads to a quantitative prediction to the mechanical response at large extensional strains. These findings clearly show how the collective inter-chain reorganization governsthe nonlinear extensional behaviors.

Keywords

Polymer physics, soft matter condensed matter, complex fluid physics, molecular dynamics simulation

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