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过冷液体非线性流变学与动力学的理论与模拟研究

摘要

过冷液体表现出复杂的动力学行为：在微观层面，其动力学特质在空间上是不均匀的，即所谓的动态不均匀性。在宏观层面，其剪切粘度随剪切速率的增加而呈幂律下降，即所谓的剪切变稀。然而两者之间的具体关联尚不明确。通过在二维、三维中几类不同体系进行模拟分析，我们发现剪切变稀与动态不均匀可以通过局部弹性来定量地联系起来，这种局部弹性体现为对剪切产生弹性响应的瞬态团簇。当这些团簇发生大规模屈服后，紧接着就会出现动态不均匀性，其由剪切转变去引发，并由弹性介导的相互作用促进。基于这一物理图景，我们找到了一个将剪切变稀与动态不均匀性的特征长度联系起来的标度关系。

关键词

过冷液体；动态不均匀；剪切变稀；分子模拟

Abstract

Supercooled liquids exhibit complicated dynamical behaviors: At the microscopic level, the dynamics is heterogeneous spatially, known as dynamic heterogeneity. At the macroscopic level, the shear viscosity decreases as shear rate increases with a power law, known as shear thinning. The relation between these two universal dynamical phenomena remains elusive. With simulations of several model liquids in two and three dimensions, we show that they are quantitatively bridged by localized elasticity embodied as transient clusters that elastically respond to shear. Prominent dynamic heterogeneity emerges right after the massive yielding of these clusters, which is initiated by shear transformation zones and facilitated by elasticity-mediated interaction. With this picture, a scaling law relating shear thinning to the characteristic length of dynamic heterogeneity is found.

Keywords

supercooled liquids; dynamical heterogeneity; shear thinning; molecular simulation

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