Microstructure Clustering in Multiphase Materials: The role of dimensionless temperature and surface fraction

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The significant development and intensified use of composite materials (reinforced plastics, extruded materials and mechanically blended thermoplastics) over the last 30 years has provided the impetus for intense research on their processability as well as on the durability and properties of the final products. In disperse multiphase systems, the dispersion/distribution of particles (microstructure) is regarded as a key factor, both affected by processing and in its turn determining performance. Among many microstructural features, clustering, that is, the tendency of dispersed particles to agglomerate forming clusters of various sizes is considered of primary significance. Our purpose in this study is both, to understand the evolution of clustering with dimensionless temperature and surface fraction parameters, and also to investigate its influence on effective properties, namely effective diffusivity and permeability. The microstructures we use are generated using Monte-Carlo simulations of Lennard-Jones fluids. During the MC process, each particle gets displaced, randomly and sequentially, by the small amount relative to its original position. The interaction of each displaced particle is checked against every other particle, and particles are subject to attractive/repulsive forces, described by the Lennard-Jones potential, defined as $u(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$, while they are also subject to thermal motion, expressed by a dimensionless temperature T. Earlier research has shown that a microstructure generated by the aforementioned procedure would evolve to different equilibrium states, depending on T. However, no formal, quantitative assessment of this was offered (TD Papathanasiou 2009). In this study, the main parameter quantifying the clustering is the standard deviation of normalized Voronoii areas σ obtained by applying Voronoii tessellation method on particles positions using the information on mean local field of Voronoii areas (Sumbekova 2017). Monte-Carlo simulations generated the microstructure equilibrium states for a range of surface fraction ϕ and dimensionless temperature T, both varying 5 fold. Microstructural behavior in absence of clustering is estimated by $\sigma = 0.42$ obtained from MC simulations allowing same disks to start from a Random initial configuration at $T = 1.0$. The scaling of clustering levels showed the evolution with parameters ϕ and T as $\sigma = 0.1316 \times T^{-0.45} \times \phi^{-0.52}$. The effective diffusivity computed for every generated microstructure state for given parameters is evolving as $D_{eff} = 0.25 \times T^{0.0055} \times \phi^{-0.50}$ or $D_{eff} = 0.27 \times \sigma^{0.05} \times \phi^{-0.48}$. Clearly, both clustering levels and effective diffusivity are strongly dependent on ϕ whereas T variation affects more clustering than effective diffusivity; we report a weak effect of clustering on obtained effective diffusivity. We also report the scaling of permeability evolution with clustering level σ and volume fractionϕ.

[1] Sumbekova, Sholpan, Alain Cartellier, Alberto Aliseda, and Mickael Bourgoin. 2017. *Physical Review Fluids 2* 2: 024032.