Microstructure Clustering in Multiphase Materials: Particle size effect

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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 size, is considered of primary significance.

Our purpose in this study is to understand the evolution of clustering with the variation in particles size forming the microstructure.

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, such microstructural clustering is quantified using the Voronoii tessellation method. The space of particle positions transformed into such a way that a polygon of a fixed area inverse to the local concentration field of a particle is formed around each dispersed particle. The standard deviation of the normalized Voronoii areas σ is a chosen parameter to quantify the clustering level according to the procedure of using the information about mean local Voronoii field necessary to when dealing with inhomegeneous particle position field (Sumbekova 2017). For a given microstructure of surface fraction ϕ, length $L = 1$ of the computational box and varying number of particles N allows us to calculate particles diameter d as:

$$d = 2 \times \sqrt{\frac{\phi L^2}{\pi N}}$$

The evolution of clustering level σ has been seen to evolve as d^n, where *n* is estimated over the range of numerical conditions of $\phi = 0.2$; N=500-4000; $T = 0.3 - 0.8$.

[1] S.Sumbekova, A.Cartellier, A.Aliseda, M. Bourgoin. 2017. *Physical Review Fluids 2* 2: 024032
[2] TD Papathanasiou, X Chen. 2009. *Polymers & Polymer Composites* (Smithers Rapra Technology Limited) 1