Monte Carlo Simulation of Electrical Properties in Nanocomposite Networks of 2D fillers

Yubao Deng
William Sampson, Ian Kinloch, Robert Young, Mark Bissett

Henry Royce Institute and National Graphene Institute, University of Manchester, Oxford Road, Manchester M13 9PL, UK.
Yubao.deng@manchester.ac.uk

Monte Carlo simulations are used to create 2D filler networks, where polygons represent the fillers. We employ the hard-core soft-shell (HCSS) model to ensure impenetrability and simulate realistic particle interactions. Electrical conductivity is evaluated using a resistor network and Kirchhoff matrix calculations. The study investigates how percolation thresholds and scaling exponents are influenced by stacking effects and aspect ratio. The results highlight that HCSS networks exhibit higher percolation thresholds than soft polygon systems due to geometric constraints. Stacking caused by the hard-core constraint significantly influences electrical properties, as it reduces the number of direct conductive pathways and introduces contact resistance. This effect leads to an approximately 3.5 times higher percolation threshold compared to ideal fillers, emphasizing the importance of interparticle interactions in network formation. Additionally, we observe that the percolation exponent decreases as stacking increases, indicating a shift in transport behaviour due to the constrained connectivity in stacked networks.

References

[1] Pike, G. E., & Seager, C. H. (1974). Percolation and conductivity: A computer study. I. *Physical review B*, *10*(4), 1421.
[2] Garboczi, E. J., Snyder, K. A., Douglas, J. F., & Thorpe, M. F. (1995). Geometrical percolation threshold of overlapping ellipsoids. *Physical review E*, *52*(1), 819.

Figures

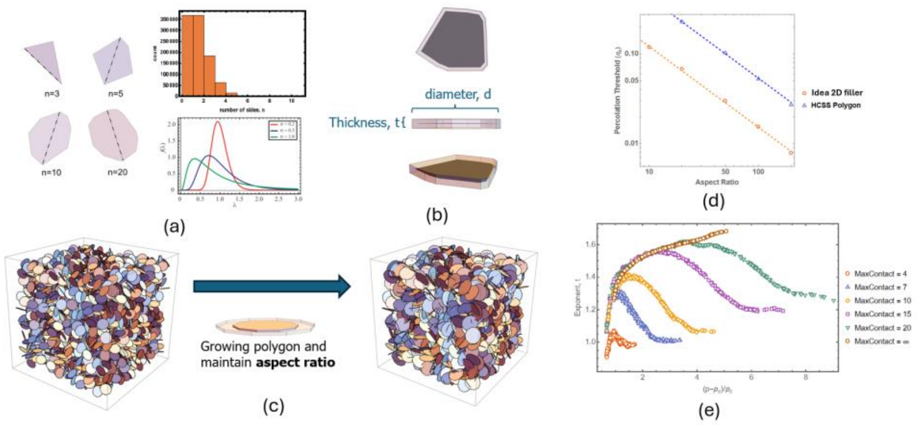

Figure 1: (a) Morphology of polygonal fillers, with histogram showing the distribution of sides and diameters. (b) Hard-core soft-shell (HCSS) model illustrating the impenetrable hard-core region (2D face) surrounded by a soft shell. (c) Growing method used to determine the percolation threshold while maintaining aspect ratio [1]. (d) Percolation threshold results as a function of aspect ratio, comparing ideal HCSS polygons and idea 2D filler [2]. (e) Dependence of the percolation exponent on filler concentration, showing how stacking influences scaling behaviour.