

Materials Science & Engineering

Master's Defense

Structural characteristics and applications of hard-particle packings via event-driven molecular dynamics simulations

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abstract

In this dissertation, we present results of our comprehensive computational studies of disordered jammed (i.e., mechanically stable) packings of hard particles, including the family of “superdisks” in 2D and ellipsoids in 3D Euclidean space. Following a very brief introduction to the hard-particle systems, the event driven molecular dynamics (EDMD) employed to generate the packing ensembles will be discussed. A large number of 2D packing configurations of superdisks are subsequently analyzed, through which a relatively accurate theoretical scheme for packing-fraction prediction based on local particle contact configurations is proposed and validated via additional numerical simulations. Moreover, we present studies on binary ellipsoid packing in 3D and briefly discuss the effects of different geometrical parameters on the final packing fraction. In the end, we provide concluding remarks and discuss several future research directions.



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