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RANDOM TESSELLATION MODELING FOR GRANULAR MICROSTRUCTURE MORPHOLOGIES

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Simulating realistic microstructure morphologies is a critical prerequisite to performing any type of high-fidelity, physics-based analysis. Microstructure morphologies of most materials are typically characterized by very complex topologies, such as grain or multi-phase inclusion shape and orientations, defect geometries, crack patterns, and many more. Further, the associated properties are usually randomly oriented and spatially correlated, which exacerbates the challenges of generating realistic virtual microstructures. For granular materials, such as metal alloys, a common approach is to model the morphological structure using a Voronoi Tessellation (VT) model [1]. A VT is defined such that a point within the tessellation is assigned to the cell that contains the minimum distance of the distances between this point and nucleation sites of all the cells. VTs are constrained to relatively regular cell shapes and, recently, Laguerre Tessellations (LT), have been utilized to capture granular structures with less uniform aspect ratios and more strongly varying number of facets (boundary components of a cell). LTs modify VTs such that a unique weight is assigned to each cell that modifies the distance comparison amongst the cells in determining the cell assignment for a point. When modeling random tessellations, VTs are defined by the cell intensity function (rate of cell nucleii per unit volume) while LTs can be described by the cell intensity function, cell boundary vertex intensity function (rate of so-called k-faces per unit volume), cell total edge length, and cell total surface area in three dimensional space [4].

There are many areas requiring development beyond the current state-of-the-art in microstructure morphology simulation. Existing models of the aforementioned random tessellation models do not take into account spatial correlation of the identified parameters, but instead only the marginal densities are matched. Spatial correlation functions, such as two-point correlation functions or lineal path functions, have been matched using indicator functions for random field models of multi-phase materials [2], but these are

extremely computationally demanding and are not directly transferable to tessellation models, which are appropriate models for granular materials. Secondly, the vast majority of existing tessellation models require cells to be convex polytopes, which prohibit the modeling of arbitrary grain boundary shapes which can exist in reality or could be sought in understanding the uncertainty in imaging techniques [3]. Ultimately, the effect of these and other microstructure characteristics has on the material properties of interest is the key relation sought. This work is framed around this last point. Specifically, the random LT model and simulation algorithm are enhanced to include spatial correlation-consistent model parameters. The effect of considering versus disregarding spatial correlation on homogenized elastic moduli of metal alloys is studied.

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