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Generation of polycrystalline microstructures using 3D-Voronoi tessellation and genetic algorithms

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The mechanical properties of solid materials are closely related to their microstructure, e.g. grain size. Therefore, the computational modelling of polycrystalline materials plays an important role in material science and engineering especially for microstructure based processes as grain growth, deformation, recrystallization and crack propagation. The goodness of the corresponding simulations often depends on the modelling of the initial polycrystalline structure.

3D-Voronoi tessellations producing convex polyhedrons from a set of random points are often used to generate polycrystalline microstructures. These polyhedrons are called voronoi cells representing the grains in a polycrystal. Unfortunately, some important properties of the generated cells don't correlate to real microstructures, e.g. the grain size distribution which is a poisson distribution instead of a log-normal distribution. Therefore, the starting points of the cells have to be changed. This is done by numerical optimization of the random distributed starting point's positions.

In this presentation, a modified genetic algorithm belonging to the class of evolutionary algorithms is developed to optimize the 3D-voronoi cells with respect to real measured grain size distribution functions. The used heuristic search strategy is easy to implement and suitable for parallel processing. These are great advantages in computational optimization. Compared to general used genetic algorithms, modified crossover and mutation functions are implemented (similar to **[1]**) to improve the global and local search phase during the genetic optimization process of the voronoi cells. These modifications guarantee a faster convergence to an acceptable solution than conventional genetic algorithms or the Monte Carlo method **[2]**.

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