

# Maximum entropy approach for statistical modeling of three-dimensional polycrystal microstructures

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Multiscale computational methods bridging models at micro scale with macro properties is a problem of practical significance since many macroscopic properties depend strongly on geometrical variability of the micro-constituents. Probability distribution functions (PDFs) providing a complete representation of microstructural variability in polycrystalline materials using limited information is difficult to obtain since this inverse problem is highly ill-posed. We use the maximum entropy principle to find a PDF of microstructures based on given information [1]. Microstructural features are incorporated into the maximum entropy framework by obtaining data either from experiments or simulations. Microstructures are sampled from the computed PDF using concepts from computational geometry and voronoi-cell tessellations. These microstructures are interrogated using homogenization techniques to evaluate the variability of non-linear macro properties [2].

## References

1. S. Sankaran, N. Zabaras, A maximum entropy approach to property prediction of random microstructures, *Acta Materialia*, in press.
2. V. Sundararaghavan, N. Zabaras, Design of microstructure-sensitive properties in elasto-viscoplastic polycrystals using multi-scale homogenization, *Int. J. Plasticity*, in press.