

# Mechanical Engineering Doctoral Defense

## Novel Hierarchical N-point Polytope Functions for Quantifying, Modeling and Reconstructing Complex Heterogeneous Materials

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### Abstract

How to effectively and accurately describe, character and quantify the microstructure of the heterogeneous material and its 4D evolution process with time suffered from external stimuli or provocations is very difficult and challenging, but it's significant and crucial for its performance prediction, processing, optimization and design. The goal of this research is to overcome these challenges by developing a series of novel hierarchical statistical microstructure descriptors called "n-point polytope functions" which is as known as Pn functions to quantify heterogeneous material's microstructure and creating Pn functions related quantification methods which are Omega Metric and Differential Omega Metric to analyze its 4D processing.

In this dissertation, a series of powerful programming tools are used to demonstrate that Pn functions can be used up to  $n=8$  for chaotically scattered images which can hardly be distinguished by our naked eyes to find or compare the potential configuration feature of structure such as symmetry or polygon geometry relation between the different targets when target's multi-modal imaging is provided. These n-point statistic results calculated from Pn functions for features of interest in the microstructure can efficiently decompose the structural hidden features into a set of "polytope basis" to provide a concise, explainable, expressive, universal and efficient quantifying manner.

The Pn functions can also be incorporated into material reconstruction algorithms readily for fast virtualizing 3D microstructure regeneration and also allowing instant material property prediction via analytical structure-property mappings for material design.

In my research, Omega Metric and Differential Omega Metric are further created and used to provide a time-dependent reduced-dimension metric to analyze the 4D evaluation processing instead of using Pn functions directly because these 2 simplified methods can provide undistorted results to be easily compared. The real case of vapor-deposition alloy films analysis are implemented in this dissertation to demonstrate that One can use these methods to predict or optimize the design for 4D evolution of heterogeneous material.

The advantages of the all quantification methods in this dissertation can let us economically and efficiently quantify, design, predict the microstructure and 4D evolution of the heterogeneous material in various fields.

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