Unsupervised Spatial Machine Learning for Phase Clustering in Nanomechanical Maps with Kernel-Averaged Mechanical Mismatch

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Abstract

This work presents an unsupervised, spatially aware machine-learning approach for improving phase identification in nanomechanical property maps of multiphase materials, such as those obtained by nanoindentation or atomic force microscopy (AFM). Conventional clustering methods based solely on elastic modulus (E) and hardness (H) often struggle to resolve distinct phases when mechanical contrast is low or when diffuse interphase regions are present [1-3].

To address this limitation, we introduce the Kernel-Averaged Mechanical Mismatch (KAMM), a spatial descriptor that quantifies local mechanical heterogeneity through neighborhood-based comparisons in the (E, H) space. Incorporating this feature into an augmented clustering space (E, H, KAMM) enables spatially informed unsupervised segmentation, improving phase separability, interphase detection, and robustness to measurement noise.

A systematic parametric analysis is first conducted on synthetic microstructures to evaluate the sensitivity of KAMM to kernel size and contrast conditions, and to assess clustering robustness and quality under controlled scenarios. The approach is then validated on experimental nanomechanical datasets, demonstrating enhanced phase discrimination and more consistent segmentation compared with conventional property-based clustering [1].

By enabling a more reliable delineation of mechanical domains, the method facilitates the generation of realistic representative volume elements (RVEs) and supports accurate extraction of phase-specific properties for ICME-oriented modelling workflows, providing a practical bridge between experimental mapping and multiscale simulation.

References

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Figures

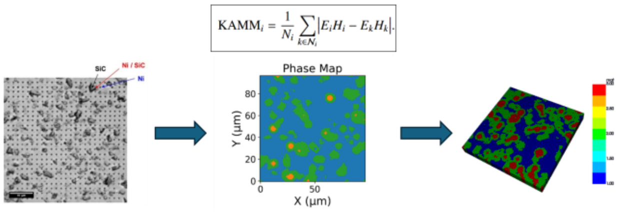

Figure 1. Workflow from mechanical characterization map to clustered phase map to RVE for mesoscale finite element modelling.

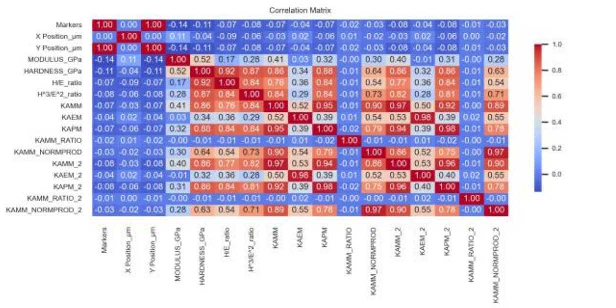

Figure 2. Correlation matrix for all mechanical features extracted from the analyzed specimen.

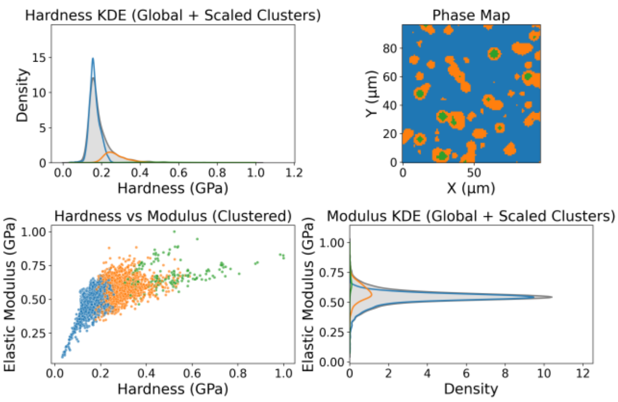

Figure 3. Agglomerative Clustering results using the full feature set including higher-order KAMM descriptors.