Identifying defects in self-assembled nanomaterials using a novel Convolutional Neural Network

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1 Problem Statement

Self-assembled nanomaterials refer to the spontaneous structural organization of materials at the nanoscale, often resulting in patterns of repeating units (Li et al. (2019); Amadi et al. (2022)). They represent a very important class of nanomaterials with significant applications, such as nanomedicine and drug delivery (Amadi et al. (2022)).

Although image-based characterization techniques for nanotechnology and nanoscience, such as Scanning Electron Microscopy (SEM), are reliable and mature, post-processing of these images to quantify structure-property relationships is an underdeveloped research area (Abukhdeir (2016)). A robust and unsupervised defect identification scheme, which does not currently exist for self-assembled nanomaterials, would greatly improve post-processing of these images.

One such solution to this problem uses a set of orthogonal basis functions called *shapelets* as kernels in convolution (Suderman et al. (2015); Akdeniz et al. (2018)). After selecting a reference region in the pattern that is defect-free, a comparison scheme called the Response Distance Method is used to compare convolutional responses at each pixel and identify areas of similarity (and dissimilarity). Algorithm limitations include (i) supervised learning and (ii) significant noise in the defect identification output.

In similar work (but not for self-assembled nanomaterials), there are few worthy attempts to identify material defects using Convolutional Neural Networks (CNNs) (Chowdhury et al. (2016); Dong et al. (2020); Boyadjian et al. (2020)). Due to limited inventory of microscopic material images, these networks either (i) partitioned existing images into smaller portions or (ii) used previously trained CNN architectures, such as AlexNET. This raises significant issues, as the partitioning of existing images does not truly introduce different topologies to the network. Furthermore, using previously trained CNN architectures 'out of the box' may not perform as intended.

2 Methodology

A novel CNN-based network trained solely on *synthetic data* will be designed from scratch to identify defects in self-assembled nanomaterials and their unique spontaneous patterns

(hexagonal, stripe, square, etc.). Thousands of pattern images that mimic self-assembly nanomaterials will be synthetically generated using methods described in Stein (1989) and Gunaratne et al. (1994). Starting with perfect patterns, these patterns will be rotated, vary in feature scale, and include combinations of perfect and imperfect patterns to model defects observed in real self-assembled nanomaterials while providing rigourous training to the network. The CNN will likely contain two stages: (i) classification of the input image into its dominant repeating pattern (i.e, hexagonal, square) and (ii) identification of defect regions. If time permits, an additional stage will include the classification of these defects in relation to fundamental material science (i.e., dislocations, disclinations, voids, etc.).

References

Nasser Mohieddin Abukhdeir. Computational characterization of ordered nanostructured surfaces. *Materials Research Express*, 3(8):082001, 2016.

Thomas J Akdeniz, Daniel J Lizotte, and Nasser Mohieddin Abukhdeir. A generalized shapelet-based method for analysis of nanostructured surface imaging. *Nanotechnology*, 30(7):075703, 2018.

Eberechukwu Victoria Amadi, Anusha Venkataraman, and Chris Papadopoulos. Nanoscale self-assembly: concepts, applications and challenges. *Nanotechnology*, 33(13):132001, 2022.

Quentin Boyadjian, Nicolas Vanderesse, Matthew Toews, and Philippe Bocher. Detecting defects in materials using deep convolutional neural networks. In *Image Analysis and Recognition: 17th International Conference, ICIAR 2020, Póvoa de Varzim, Portugal, June 24–26, 2020, Proceedings, Part I 17*, pages 293–306. Springer, 2020.

Aritra Chowdhury, Elizabeth Kautz, Bülent Yener, and Daniel Lewis. Image driven machine learning methods for microstructure recognition. *Computational Materials Science*, 123: 176–187, 2016.

Xinghui Dong, Christopher J Taylor, and Tim F Cootes. Defect detection and classification by training a generic convolutional neural network encoder. *IEEE Transactions on Signal Processing*, 68:6055–6069, 2020.

Gemunu H Gunaratne, Qi Ouyang, and Harry L Swinney. Pattern formation in the presence of symmetries. *Physical Review E*, 50(4):2802, 1994.

Li-Li Li, Hong-Wei An, Bo Peng, Rui Zheng, and Hao Wang. Self-assembled nanomaterials: design principles, the nanostructural effect, and their functional mechanisms as antimicrobial or detection agents. *Materials Horizons*, 6(9):1794–1811, 2019.

Daniel L. Stein. *Lectures in the Sciences of Complexity the Proceeding of the 1988 Complex Systems Summer School, Held June-July, 1988 in Santa Fe, New Mexico*. 1989.

Robert Suderman, Daniel J Lizotte, and Nasser Mohieddin Abukhdeir. Theory and application of shapelets to the analysis of surface self-assembly imaging. *Physical Review E*, 91(3):033307, 2015.