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Uncertainty Quantification in Polysilicon-based MEMS: a Representation Learning Comparison

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Abstract:

The production of reliable micro-electro-mechanical systems (MEMS), is significantly dependent on the ability to control the small-scale, and scale-specific properties associated to their constituent materials. This represents a challenge since manufacturing processes of MEMS are typically subjected to limited repeatability [2, 3]. In these systems, nominal geometries and material properties constitute target values, while experimentally obtained results are characterized by a scattering around these instead [8].

For the particular case of polysilicon-based MEMS, uncertainties associated with the intrinsic heterogeneity of the material have been observed to intensify with the miniaturization [5, 6, 4, 1]. Such heterogeneity can be characterized by the specific topology of the grain boundary network and the lattice orientation of each grain. Since both microstructural descriptors are ultimately governed by variables that are stochastic in nature [5], statistical approaches need to be adopted to quantify the expected scattering induced in the effective properties.

Given that the prediction of the effective properties of heterogeneous random media, like e.g. polycrystalline materials, can be computationally-intensive, data-driven approaches represent a viable alternative. The use of deep learning strategies based on artificial neural networks can be therefore envisaged due to their intrinsic capability of automatic feature extraction from large datasets, allowing for an uncertainty quantification procedure in a straightforward data-driven manner.

In this context, one of the main challenges in the implementation of effective supervised deep learning models is represented by the capability to learn representations that capture meaningful features of the data, to guarantee satisfactory generalization on unseen data during the inference stage. This aspect depends on both the availability of sufficient and representative training samples on one hand, and on the selection of an adequate model on the other, often determined by the specific input/output data profile.

Moving from our previous results collected in [7], in this work we focus on the latter aspect and propose a comparison between two different representation learning approaches for the task of achieving accurate mappings between a set of digitally generated images, representing typical microstructures of epitaxially-grown polysilicon thin-films, and their corresponding effective mechanical properties, in terms of the relevant elastic moduli. Specifically, a comparison is established between the performance of a regression model based on a convolutional neural network (CNN) as feature extractor, and that yielded by a regression model based on an autoencoder (AE) architecture instead.

In a first set of experiments, a series of CNN-based regression models are trained for the above-mentioned microstructure-property mappings. We show the influence of the model size on the quality of the mappings. We further discuss the influence of the main architectural hyperparameters on the representation learning capabilities, and their optimal configuration in relation with the attributes of the input data.

We then explore whether a regression model, based on features extracted from the low dimensional space projection of the input images using an effectively trained generative model, could be linked to an enhanced generalization in comparison to the one using a CNN backbone. For this goal, we propose the use of an AE neural network to learn a compressed representation of the raw input data (images) in a

first phase. Once the AE model is trained, the reconstruction aspect of this model is discarded, and the vector of latent space variables is used as the input feature vector of a supervised learning model based on a standard multilayer perceptron (MLP). The MLP is then trained on a second phase, to provide the mapping of the effective moduli.

The representation learning capabilities of the proposed AE-based regression model are evaluated indirectly, by comparing its performance with that of the CNN baseline. Some preliminary results are here reported, and the performance of the two different approaches is discussed.

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Short biography – Bachelor in Mechanical Engineering at Universidad de Costa Rica where he won a scholarship to complete his post-graduate studies at Politecnico di Milano, Italy. Graduated from Master in Materials Engineering and Nanotechnology (2020), same year he started the Ph.D. in Structural Seismic and Geotechnical Engineering. Research oriented to the application of deep learning algorithms for microstructure-property mappings, with particular focus on the industry of polysilicon-based MEMS. . . .