Introduction to artificial neural networks and their applications in structural analysis and modeling of polycrystalline materials

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Abstract

A broad range of engineered as well as natural materials exhibit polycrystalline microstructures, i.e., they consist of a large number of crystals (also called grains) with different atomic lattice orientations arranged in a space-filling manner. The macroscopic (functional) properties of these materials are often strongly influenced by their internal grain architecture, typically observed in experimentally acquired 2D/3D microscopic image data.

Artificial neural networks (ANNs) have become powerful tools for extracting information from this type of image data: convolutional neural networks can segment grains in 2D/3D image data, which in turn facilitates subsequent analysis and modeling workflows [1]. Beyond segmentation, ANNs can be deployed as generative models. For example, generative adversarial networks (GANs) can synthesize image data that exhibits grain architectures that are similar to experimentally observed ones [2]. Such artificially generated microstructures can serve as input for further numerical simulations, enabling virtual materials testing and thereby reducing experimental effort. Moreover, generative approaches can help overcome the limitations of 2D imaging techniques by learning to generate 3D images of grain architectures that are consistent with 2D observations.

Besides representing grain architectures as discretized image data, grain architectures can also be described in a space-continuous manner using tessellation models, in particular, power diagrams. Such representations are advantageous, as they are typically defined by relatively few parameters. Methods from ANNs can contribute to this representational framework by enabling the efficient fitting of power diagrams to segmented image data [3]. In particular, by leveraging programming libraries that enable automatic differentiation, gradient-based optimization can be used to identify parameters of power diagrams that best approximate the grain architectures observed in image data. Beyond deterministic fitting, differentiable implementations of power diagrams enable ANN-guided generative modeling [4]. ANNs can be deployed to learn the probability distribution of power diagram parameters instead of directly learning the distribution of high-dimensional image data, which would be the common approach in conventional GAN-based modeling. The combination of power diagrams with ANNs, induces geometric regularization, as generated samples are constrained to physically reasonable morphologies by the chosen type of power diagram. In particular, this approach facilitates learning the probability distribution of 3D grain architectures from just a few 2D images, thereby reducing the need for costly and time-intensive 3D experimental characterization.

References

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