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Mechanical and morphological analysis of silica aerogels using a reinforcement learning approach

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Silica aerogels are ultralight materials with a highly open-porous microstructure characterized by very low density, thermal conductivity, and sound velocity. Their fractal morphology has a significant impact on their physical properties. Using the diffusion-limited cluster-cluster aggregation (DLCA) method, microstructures correlating with the fractal properties of aerogels can be created, which allow predicting their material behavior [2]. Although this modeling approach is time-consuming, it generates many microstructure datasets. Based on these datasets, artificial neural networks can successfully map the DLCA input variables to target material properties as, for example, the fractal dimension of the microstructure [1].
In this work, this initial solution is extended by a reinforcement learning approach to enable the development of aerogels with specific physical properties by reverse engineering. An intelligent agent takes actions in an environment for optimizing Young's modulus and the fractal dimension for the desired aerogel microstructure. This method does not dependent on the prior knowledge of the desired input space and finds an optimal solution based on a reward function. The material behavior of the generated structures is determined by finite element analysis of representative volume elements. The ansatz is evaluated for specified target properties for Young's modulus and the fractal dimension. Good accuracy in the prediction of material behavior is obtained.

References

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