Dimensionality Reduction of Nanoparticle Reinforced Ice Microstructures

The use of machine learning techniques for materials science has gained significant interest in recent years due to their potential to accelerate the discovery and optimization of new materials. However, one of the challenges in this field is the high dimensionality of materials microstructures or properties, which can hinder efficient analysis and modeling. In this study, we propose an approach for reducing the dimensionality of nanoparticles-reinforced ice microstructures using autoencoders, a type of deep learning model that can learn compressed representations of high-dimensional data. By reducing the dimensionality of the data, we can accelerate multi-scale modeling and simulation of the material, enabling more efficient design and optimization. We demonstrate the effectiveness of our approach by applying it to a dataset of nanoparticles-reinforced ice microstructures represented as two-dimensional coordinates and corresponding materials properties. Our results show that the autoencoder can effectively reduce the dimensionality of the data while maintaining the essential information with an error rate of 0.2%. Overall, our study demonstrates the potential of using autoencoders for dimensionality reduction of materials microstructures or properties, with implications for accelerating materials discovery and optimization. The proposed approach could be extended to other complex materials systems, enabling more efficient modeling and simulation of these materials, and ultimately accelerating the development of advanced materials for various applications.