frontiers | Frontiers in Materials

TYPE Editorial
PUBLISHED 17 April 2023
DOI 10.3389/fmats.2023.1198344

OPEN ACCESS

EDITED AND REVIEWED BY
Douglas Soares Galvao,
State University of Campinas, Brazil

*CORRESPONDENCE
Shaoping Xiao,
shaoping-xiao@uiowa.edu

†These authors have contributed equally to this work

RECEIVED 01 April 2023
ACCEPTED 11 April 2023
PUBLISHED 17 April 2023

CITATION
Xiao S, Bordas SPA and Kim T-Y (2023), Editorial: Deep learning in computational materials science.
Front. Mater. 10:1198344.
doi: 10.3389/fmats.2023.1198344

Editorial: Deep learning in computational materials science

Shaoping Xiao[1*†], Stéphane Pierre Alain Bordas[2†] and Tae-Yeon Kim[3†]

[1]Department of Mechanical Engineering, University of Iowa, Iowa City, IA, United States, [2]Doctoral Program in Data and Computational Sciences, University of Luxembourg, Luxembourg, Luxembourg, [3]Civil Infrastructure and Environmental Engineering, Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates

KEYWORDS

deep learning, convolutional neural networks, generative adversarial network, materials science, modeling and simulation

Editorial on the Research Topic
Deep learning in computational materials science

Riding the current wave of artificial intelligence (AI), many engineers and scientists have adopted machine learning (ML) and deep learning (DL) as powerful tools in various science and engineering disciplines, including materials science. Utilizing artificial neural networks (NNs), DL is one of the most effective, supervised, time-efficient, and cost-efficient ML approaches. It has been successfully used in various computational materials science research topics, such as developing potential functions for molecular dynamics, predicting the mechanics of materials, optimizing material and structural design, and promoting novel multiscale modeling and simulation. Moreover, DL enhances the data-driven approach in the materials science research community via big data analyses and image processing. This Research Topic aims to unite researchers to share insights into AI in current research projects and promote DL applications in computational materials science.

Machine learning uses statistical models to analyze data and draw inferences from its pattern. Particularly, supervised learning models learn the relationship between the input features and the output targets without explicit instructions. As a subset of ML, DL employs NNs to find appropriate representations from data for progressively good performance. In this Research Topic, Deshpande et al. proposed three types of NN architectures to learn non-linear deformation efficiently to accelerate simulations in solid mechanics. The considered NN frameworks were based on convolutional neural networks (CNNs), multichannel aggregation networks (MAgNET), and attention-based neural networks, respectively. In addition, they employed two benchmark examples of largely deformed soft bodies and demonstrated the capabilities of the proposed methods to replace high-fidelity computational models in computational materials science.

Since CNNs have been successfully utilized in image processing, they were also recently employed in computational materials science to quantify material (especially composite materials) microstructure for predicting material properties. Two articles in this Research Topic have promoted the applications of CNNs to material behaviors at the microscale. First, Bachmann et al. presented CNN-based DL segmentation of prior austenite grains from Nital etched light optical micrographs. Such segmentation can determine the prior grain sizes based on information that cannot be automatically extracted from optical micrographs. They demonstrated that the proposed framework was accurate, robust, and efficient. In addition,

their methods can be extended to studying recrystallization or grain growth in austenite. In another work, Khurjekar et al. developed a CNN-based predictive model that could automatically and accurately classify textured microstructures without knowledge of crystallographic orientation. Mainly, CNNs were used to extract high-order morphological features to distinguish textured microstructures from untextured ones. They concluded that CNNs could identify the subtle morphological patterns that result from texture, especially at the early stages of grain growth.

The recent achievement in the DL community benefited materials science research too. In this Research Topic, Barrera et al. proposed an audio-visual generative adversarial network (GAN) to generate artificial architectures mimicking the native ones of complex cartilaginous tissues. The GAN used a dataset, including traditional imagery and sound generated from each image. The authors found that the audio information could provide more features, uncovering some hidden characteristics not visible with images only. According to their demonstration, the GAN-generated dataset based on the downsized ones performed better than the compressed images in recognizing microstructures from the original images.

Four articles in this Research Topic demonstrated that DL techniques have enormous potential to revolutionize the field of materials science, especially in modeling and simulation. As more researchers explore the applications of DL in materials science, we can expect to see even more exciting advances in this field shortly.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Publisher's note