

Machine Learning for Designing Stretchable Carbon Nanostructures

Helena Hepler, James Clarkston

Department of Mechanical Engineering, Kennesaw State University, Marietta, Georgia 30060

In this research study, we employ machine learning algorithms to perform molecular dynamics simulations for graphene-like 3D carbon nanostructures. The accuracy of molecular dynamics simulation largely depends on the quality of inter-atomic potential that is pre-defined before executing molecular dynamics simulations. Discrepancies exist among the simulation results for carbon-based nanostructures such as graphene because of this limit. Machine learning is an application that enables a system to learn and improve based on experience and patterns rather than explicit instructions. Instead of using pre-defined interatomic potentials, force information among carbon atoms in the structures are machine learned during the time evolution of molecular dynamics simulations. Researchers have successfully used machine-learned inter-atomic potentials for predicting mechanical properties of graphene which is an exciting wonder carbon-based nanomaterial. Here, we employ the machine learned interatomic potentials developed for graphene for predicting thermal transport properties of 3D carbon nanostructures that are comprised of graphene floors and carbon nanotube pillars. Convolutional neural network algorithm is used to attain a precise molecular dynamic simulation which predicts the thermal properties of the 3D carbon nanostructures. This demonstrate the potential power of machine learning in finding an accurate solutions for thermal properties for 3D carbon nanostructures close to the precision of that of the molecular dynamics simulations at a fraction of iterations that would be required for a purely molecular dynamic experiment based approach; where no pre-defined interatomic potentials are known. Custom MATLAB programs and Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) are used to conduct the simulations in this report. 3D carbon nanostructures are expected provide exciting the thermal/mechanical properties that can be found in graphene. The results obtained in this research will accelerate the development of more advanced nanomaterials such as 3D carbon nanostructures by improving the accuracy of the simulations of their material properties.