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Thermal and Mechanical Properties of Polymers using Molecular Dynamics

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ABSTRACT

Polymer systems have gained attention during the past years because of their technological and industrial applications. Simulations, particularly molecular dynamics, are very useful for exploring properties of amorphous polymers, without using experiments. Our goal is to create a readily-available tool that will perform MD simulations in order to get thermal and mechanical properties (Glass transition temperature, Young Modulus) of the polymers. The work that has been done will be part of a tool to help people to learn about polymer properties including Glass Transition Temperature. We model some polymers at a scale of 10,000 atoms. The tool uses LAMMPS to perform MD simulations, with the DREIDING force field. The polymer structures were obtained using Polymer Modeler and the post processing is done using a created Python code. Thus far the problems in modeling the glass transition temperature have been many, but we have been able to model it to a relatively good degree. This tool is intended to be open for general use on NanoHUB. In the future, this tool will likely be expanded to cover further physical properties of further polymers.

KEYWORDS

Polymer, simulation, molecular dynamics, LAMMPS, glass transition, nano, materials