Introduction to Molecular Dynamics Simulation of Carbon Nanotubes (CNTs) using LAMMPS

Carbon Nanotubes (CNTs) are a class of nanomaterials with extraordinary mechanical, thermal, and electrical properties, making them critical in various applications ranging from electronics to composite materials. CNTs, which consist of rolled-up sheets of graphene, exhibit unique one-dimensional structures that confer high strength, flexibility, and excellent conductivity. This makes them highly attractive for advancements in nanotechnology, materials science, and engineering.

In the realm of computational materials science, Molecular Dynamics (MD) simulations offer powerful insights into the atomic-scale behavior of CNTs, allowing researchers to study their properties under various conditions such as strain, temperature, and external forces. Using MD simulations, scientists can predict the mechanical stability, fracture behavior, and thermal conductivity of CNTs, which are crucial for their implementation in nanoscale devices and systems.

LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) is one of the most widely used open-source MD software tools, offering robust capabilities for simulating a wide range of materials, including CNTs. The ability to model interatomic potentials, run large-scale simulations efficiently, and extract detailed atomic trajectories makes LAMMPS an invaluable tool for CNT research.

In this work, we conduct a Molecular Dynamics simulation of a (10,10) single-walled carbon nanotube (SWCNT) using LAMMPS. The simulation focuses on understanding the atomic interactions within the nanotube structure under specific boundary conditions. A key objective of this study is to visualize and analyze the atomic arrangements and how the CNT structure behaves under various simulation conditions.

To achieve this, a LAMMPS input script and an accompanying data file containing the atomic coordinates and simulation box dimensions were created. The initial CNT structure contains 100 atoms, and the simulation box was defined to encapsulate the nanotube while minimizing excess empty space. Post-simulation visualization and analysis were conducted using OVITO (Open Visualization Tool) to ensure accurate representation of the CNT and analyze the results.

This simulation provides a stepping stone for more advanced studies on CNTs, including their interactions with other materials, mechanical response under deformation, and thermal conductivity at the nanoscale. Through this approach, we aim to contribute to the growing body of knowledge on carbon-based nanomaterials and their potential applications in next-generation technologies.