STUDY OF THE MECHANICAL PROPERTIES OF WSE2 NANO-ORIGAMIS WITH REACTIVE MOLECULAR

Érick dos Santos Morais - Universidade de Brasília (UnB) - ericksantosmorais@gmail.com
Marcelo Lopes Pereira Júnior - Universidade de Brasília (UnB) - marcelo.lopes@unb.br
Luiz Antônio Ribeiro Júnior - Universidade de Brasília (UnB) - ribeirojr@unb.br

The research addresses the study of the mechanical properties of WSe2 Nano-Origamis through reactive molecular dynamics. Using computational simulations with the LAMMPS software and the reax force field, we investigate the mechanical behavior of molecular kirigamis of WSe2. Kirigami is a process of creating patterns and shapes by cutting, stretching, or twisting materials. In molecular systems, kirigamis can be generated by manipulating the atomic structure of a material to create new molecular arrangements. Our study focuses on investigating the mechanical behavior of molecular kirigamis of WSe2 and their impact on the material's fracture patterns and elastic properties. To minimize modeling stresses, we equilibrate the system with the NPT ensemble for 100 ps and then apply uniaxial tension with the NVT ensemble at 300 K. We simulate the temporal evolution of atoms and molecules in the system using the Newton equations of motion and the Velocity-Verlet algorithm. Similar studies have been conducted on kirigamis of graphene and MoS2, and this work builds on these previous findings to investigate WSe2. Our findings contribute to the fundamental understanding of WSe2, open up new avenues for material science research, and emphasizing the importance of utilizing advanced computational methods to investigate the properties of materials and their potential technological applications.

Palavras-chave: Transition metal dichalcogenides. Molecular dynamics. LAMMPS Software.