Investigating the Mechanical Behavior of Molecular Kirigamis of WSe2 using Molecular Dynamics Simulations

Erick Dos Santos Morais[1], Marcelo Lopes Pereira Júnior[2], Luiz Antônio Ribeiro Júnior[1]

[1]Universidade de Brasília (*Institute of Physics*) , [2]Universidade de Brasília (*Faculty of Technology Department of Electrical Engineering*)

e-mail: 221010407@aluno.unb.br

Transition metal dichalcogenidesis study, we investigate the mechanical behavior of molecular kirigamis of WSe2 using molecular dynamics simulations with the LAMMPS software [1] and the reax force field [2]. Kirigami is a process of creating new 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 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 [3], 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 emphas the importance of utilizing advanced computational methods to investigate the properties of materials.

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