Method for visualization of defects in Graphene

By: Koren Shreiber, MSc student

Supervisor: Dr. Joan Adler
Molecular Dynamics (MD) is a computational method to determine the trajectories of atoms in phase space according to Newton’s equations of motion (F=ma). The interaction energy is calculated according to atom position only, using an effective interatomic potential. We do not solve quantum equation every time step.
What is LAMMPS?

- LAMMPS – Large-scale Atomic/Molecular Massively Parallel Simulator – MD simulation tool, designed to run efficiently on parallel computers.
- LAMMPS is distributed freely under the terms of the GNU Public License (GPL)

History:

- LAMMPS development began in the mid 1990s. The goal was to develop a large-scale parallel classical Molecular Dynamics (MD) code. The coding effort was led by Steve Plimpton at Sandia.
- A final F77 version was released as LAMMPS 99 (1999).
- A final F90 version was released as LAMMPS 2001.
- The current LAMMPS is a rewrite in C++ and was first publicly released as an open source code in 2004.
- It also includes features from older parallel MD codes written at Sandia, namely ParaDyn, Warp, and GranFlow.
This script builds an infinite Ni fcc lattice with a lattice parameter of 3.52 Å ([111] direction is the z-axis).

Then the simulation cell is relaxed for 5000 time steps.

Nph allows the cell size to change in order to relax the hydrostatic stresses to zero.
Graphene is a substance made of pure carbon, with atoms arranged in a regular hexagonal pattern similar to graphite, but in a one-atom thick sheet.

- Potential applications:
  - Lightweight, thin, flexible, yet durable display screens
  - Electric circuits
  - Solar cells
  - Various medical, chemical and industrial processes.
Defects in Graphene

- Defects are missing carbon atoms in the lattice.
- The atoms that are located around the defect (neighbors) reorganize.
- Order parameters to identify defects by:
  - The number of atom neighbors is different than 3.
  - The angle between atoms interactions is different than $120^\circ$.
- Visualization of defects (using coloring method) with AViz
Questions?