Progress report on M.Tech project for the month of August 2021

Project title: Design aspects of Lithium-ion battery for electric vehicles.

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1. Last month's progress: I had finished comparing all the different available cathode electrodes which are being used in the Lithium-ion battery currently. The details are as follows:

Battery	Energy Density (Wh/kg)	Cyclability (Cycles)	Advantages	Disadvantages
LCO	150–200	500–1000	Technologically maturity, Low-self discharge, High discharge voltage	High cost, low inherent safety
LMO	100–140	1000–1500	High safety, Cobalt-free, hence non-toxic	Low energy density
LFP	90–140	up to 2000	High safety	Low energy density
NCA	200–250	1000–1500	Low cobalt content	Capacity fade at elevated temperature
NMC	140–200	1000–2000	Low cobalt content	Safety issues in Ni-rich batteries

Lithium Nickel Manganese Cobalt Oxide (NMC), Lithium Iron Phosphate (LiFePO4) and Lithium Manganese Oxide (LMO) stand out as being superior among these candidates.

2. Objectives for this month: Build the structure (unit cell) of Lithium Manganese Oxide in LAMMPS.
3. Plan of action: Study the structural properties of Lithium Manganese Oxide and the potential files to be used for the same in LAMMPS. Since LMO has 3 different atoms, separate potential files would be needed for each inter-atomic and intra-atomic combination.
4. Progress: Understood the basic working of LAMMPS by simulating the deformation of a Cu atom under uniaxial compressive loading using meam potential. The simulation results were visualised with the help of OVITO. It makes molecular dynamics simulations visual. It offers a wide range of basic visualization and analysis functions. These operations, which are all configurable, will then be applied to the simulation data in real-time by the software. The outcome of the data pipeline is finally displayed on the screen.

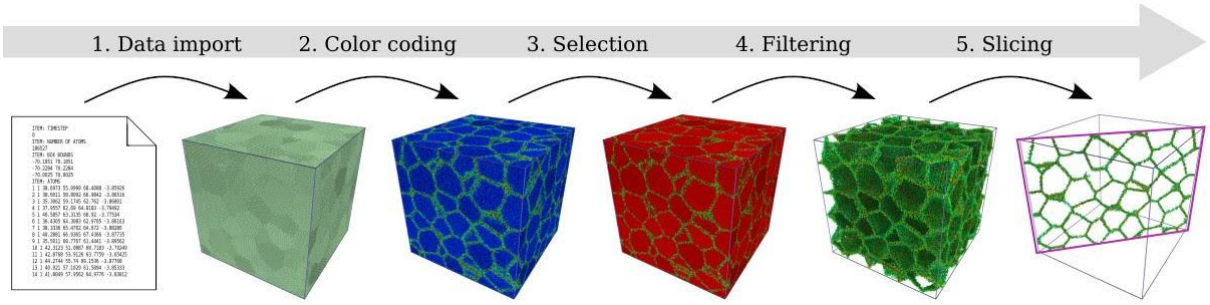

Figure 1. The basic pipeline of visualization in OVITO. Picture reproduced from [1].

Colour coding was set to colour based on the centre symmetry and then adjusted this range to go from zero to five. What the centre symmetry does is, indicates how close to a perfect lattice structure each atom is in so the dark purple atoms have a centre of symmetry very near zero and that essentially means that it is nearly in a perfect crystal structure so all the atoms around it are in the right places. The atoms with lighter colours have a relatively high centre symmetry which means they are vibrating or are somewhat out of their perfect crystal structure and their vibrations are why we see this variation in colours even before we started deforming it. As we simulate by clicking the play button and we see it compress. We start to see some very high Center symmetry values and this indicates a dislocation and they happen in these very specific planes. So those are the dislocations forming and then we can see it just gets squashed and squashed and then comes back a little bit.

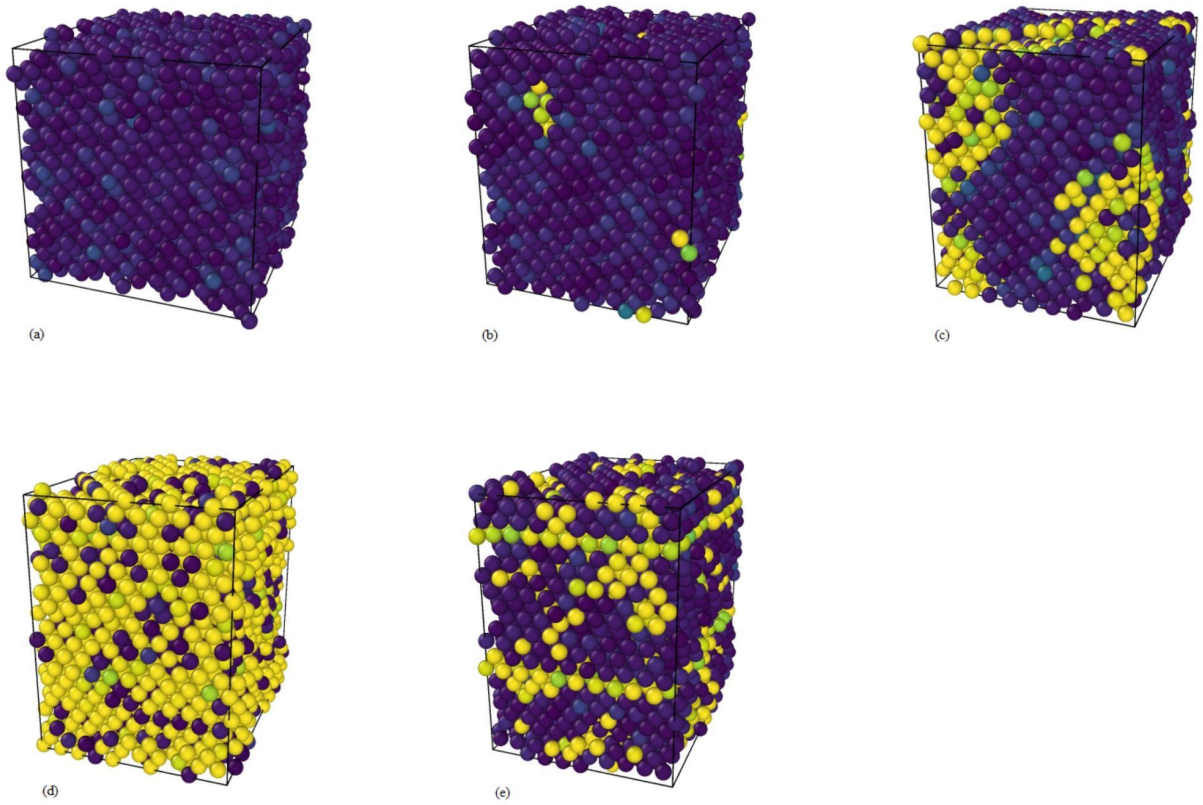

Figure 2. Simulation results for Cu compression: (a) the unit cell at 1st second, (b) the unit cell at 8th second, (c) the unit cell at 9th second, (d) the unit cell at 14th second and, (e) the unit cell at 16th second.

5. Future plans: To build on the knowledge gained by this example simulation in LAMMPS and OVITO to simulate the target material which is Lithium Manganese Oxide and study how the structure behaves in the presence of an electric field.

References:

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