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

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

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1. *Last month's 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.

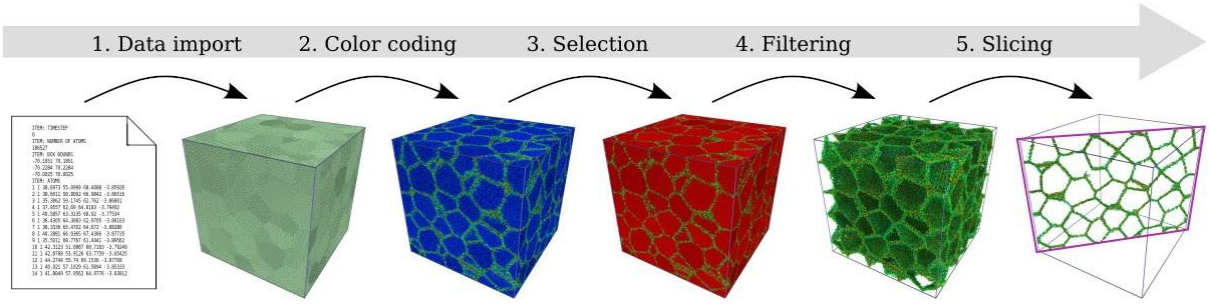

Figure 1. The basic pipeline of visualization in OVITO. [1]

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.

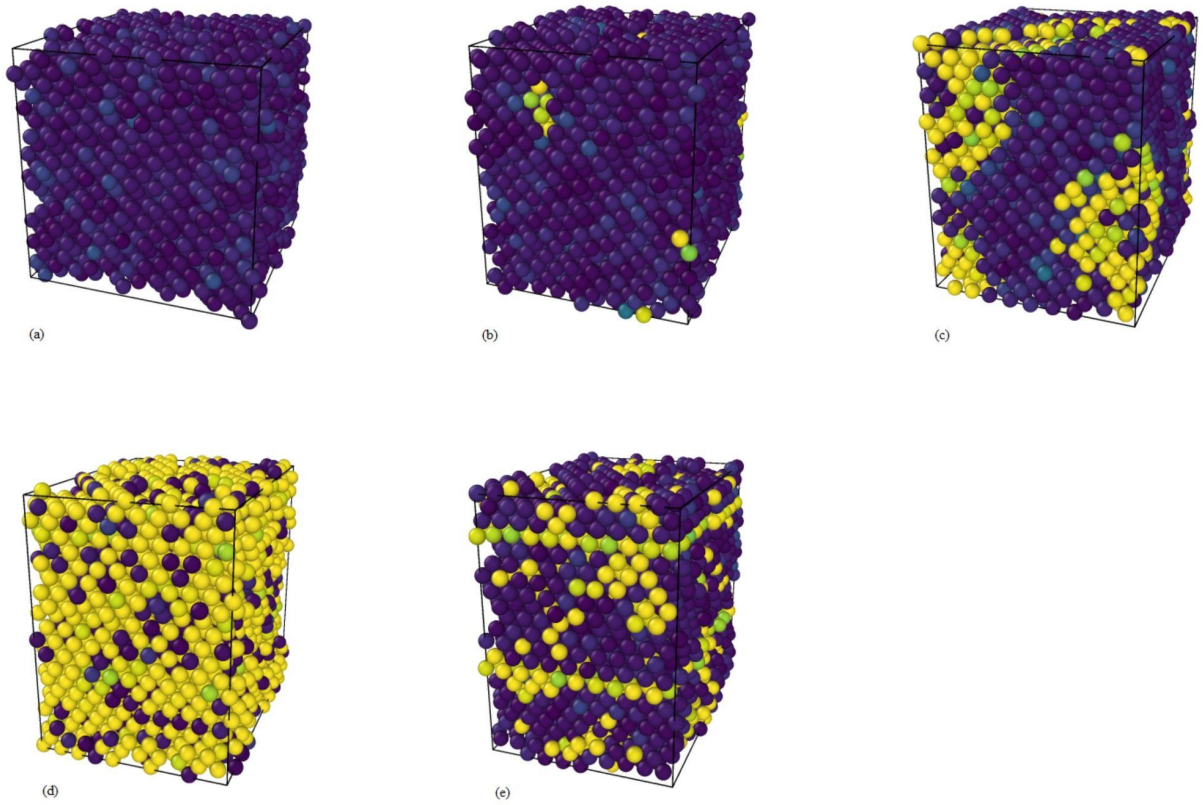

Figure 2. Simulation results for Cu compression: (a) the unit cell at 1st second, (b) the unit cell at 8th second, (c) the unit cell at 9th second, (d) the unit cell at 14th second and, (e) the unit cell at 16th second.

2. *Objectives for this month*: Build the structure (unit cell) of LFP and NMC in VESTA. Import the unit cell of LMO in LAMMPS using Atomsk and simulate the structure in LAMMPS.

3. *Plan of action*: Study the structural properties of LFP and NMC and make their unit cell in VESTA which would require all the structural properties like space group, α,β,γ and lattice type. To import the LMO unit cell in LAMMPS, a software called Atomsk would be used.

4. *Progress*: Made the unit cell of LMO in VESTA.

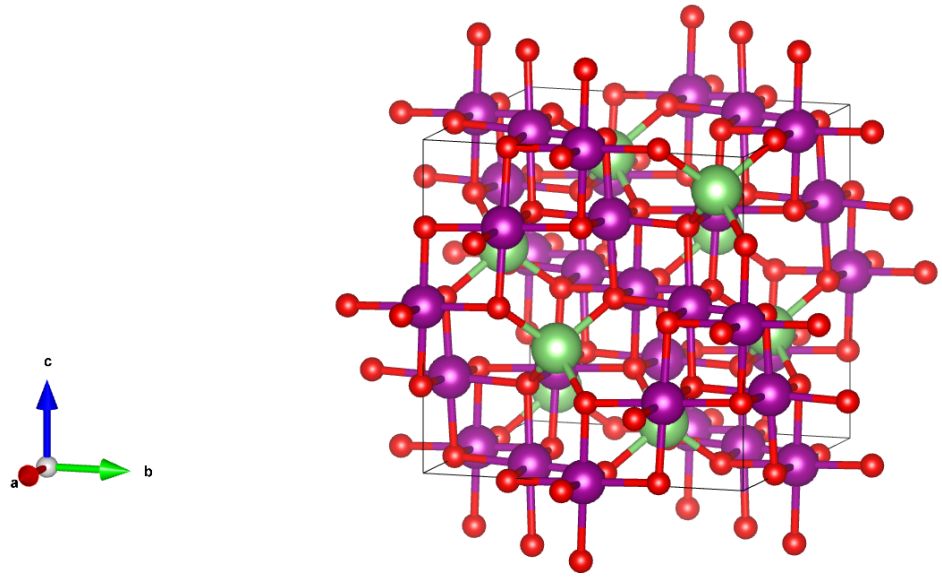

Figure: Unit cell of Lithium Manganese Oxide made using “VESTA”

Lattice type: F
Space group name: F d -3 m
Space group number: 227
Setting number: 2
Lattice parameters:

a	b	c	alpha	beta	gamma
8.24500	8.24500	8.24500	90.0000	90.0000	90.0000

Unit-cell volume = 560.495283 Å^3
Number of polygons and unique vertices on isosurface = 0 (0)
137 atoms, 218 bonds, 39 polyhedra; CPU time = 13 ms

5. Future plans: To import LMO in LAMMPS using Atomsk and then work in LAMMPS with the LMO structure and simulate it under different loads and conditions to calculate SOC based mechanical properties. Make the unit cell of LFP and NMC afterwards.

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[4] Mohamed, Nourhan, and Nageh K. Allam. "Recent advances in the design of cathode materials for Li-ion batteries." RSC Advances 10, no. 37 (2020): 21662-21685.
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[7] Asadi, Ali, Seyed Foad Aghamiri, and Mohammad Reza Talaie. "Molecular dynamics simulation of a Li x Mn 2 O 4 spinel cathode material in Li-ion batteries." RSC Advances 6, no. 116 (2016): 115354-115363.
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