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ME 395
Homework 2
Due 10/5/2021

Overview
The goal of my ongoing research projects is to decipher how oxidation levels affect the mechanical response of multi-layered graphene oxide (MLGO). GO has two types of oxidization: hydroxyl groups and epoxide groups. The chemistry of each group certainly effects the mechanical properties of MLGO, but functionalization is difficult to control in a laboratory setting. Molecular dynamics simulations can fill this knowledge gap by controlling the exact proportions of oxide groups and examining the mechanical outcomes.

Module 1: Multimodal data generation and collection
MLGO systems are generated from a MATLAB script. Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) is used to perform molecular dynamics simulations on the systems, where tensile tests are simulated. The outputs are controlled and collected as needed.

Module 2: Extraction of mechanistic features
LAMMPS is capable of calculating and outputting many mechanical quantities including energies, forces, pressures, densities, bond breakages, and more. Most of the properties I am interested in (elastic modulus, toughness, ultimate strength) can be retrieved from stress-strain curves. While LAMMPS does not output stress-strain curves directly, I can have it compute the strain from distance travelled and the stress from pressure and then write the data to an output file.

Module 3: Knowledge-driven dimensional reduction
While the effects of oxidation are also by distribution and environment, I choose to first consider the percentage present as this is likely to have the largest impact on the mechanical performance. As such, the factors to be considered are hydroxyl oxidation percentage, epoxide oxidation percentage, and total oxidation percentage.

Hydroxyl oxidation %	0	0	0	0	10	10	10	10	20	20	20	30	30
Epoxide oxidation %	10	20	30	40	0	10	20	30	0	10	20	0	10
Total oxidation %	**10**	**20**	**30**	**40**	**10**	**20**	**30**	**40**	**20**	**30**	**40**	**30**	**40**

Note that there is no 0% oxide case as this model was not designed with that in mind. Also note that the oxide concentration does not exceed a total of 40% as the model starts misbehaving.

Module 4: Reduced order surrogate models
Since there is no feasible way to precisely control the oxidation levels of MLGO in physical experiments, there are currently no mathematical models to my knowledge. From intuition and my readings, I expect the mechanical responses to increase linearly with the degree of oxidation before plateauing once the effect is maximized (if that point is reached in ≤40% oxidation).

Module 5: Neural networks for regression and classification
Once all the data is collected, precise relationships between the oxidation levels can be elucidated through regression. In the past I have used Python for curve fitting and lately I've been learning R for regression analysis, but I expect I will learn how to combine these with neural networks in this course (I currently have no idea how to use neural networks).

Module 6: System and Design
Once this analysis is complete, the relationships established between oxidation levels and MLGO mechanical performance can be used by my funding source to guide adjustment of their manufacturing techniques so that the ballistic penetration resistance of their structure is maximized.