**MSE 551**

**HW#3**

1. Use the relation between Cp, α and Cv to calculate Cv

Ran the NPT simulation for aluminum using a 10X10X10 FCC structure at 250, 300 and 350K for temperatures. Transferred the data to Excel and found where the data was at around equilibrium and averaged the points for temperature, enthalpy and volume, and using this solved the above equation, detailed in the Excel file. The average Cv I found was 1.199762(eV/K).

1. Calculate Cv of Al using an NVT (at 300K and the volume corresponding to 0 pressure) ensample and compare it to Q1 (start with the final structure from the NPT run.

Ran the NVT simulation using the final structure for the 300K structure from the NPT simulation, again for three temperatures. Energy vs. volume was plotted and the Cv was calculated to be 1.0355(eV/K). So the NVT simulation appeared to give us a smaller Cv than the NPT simulation.

1. Run an NVE simulation (start with the NVT structure). Dump the velocity of one atom every 10 fs. Then calculate the velocity autocorrelation function (VACF). Calculate the Fourier transform of the VACF to get the vibrational density of states (VDOS).

Ran the simulation gathering data every 1(fs) using the vacf function in lammps, sent this to excel and gathered the data for every 10(fs) and exported it to MATLAB, then ran a function to convert the data to plot the fourier transform of the vacf vs. frequency, shown below.

