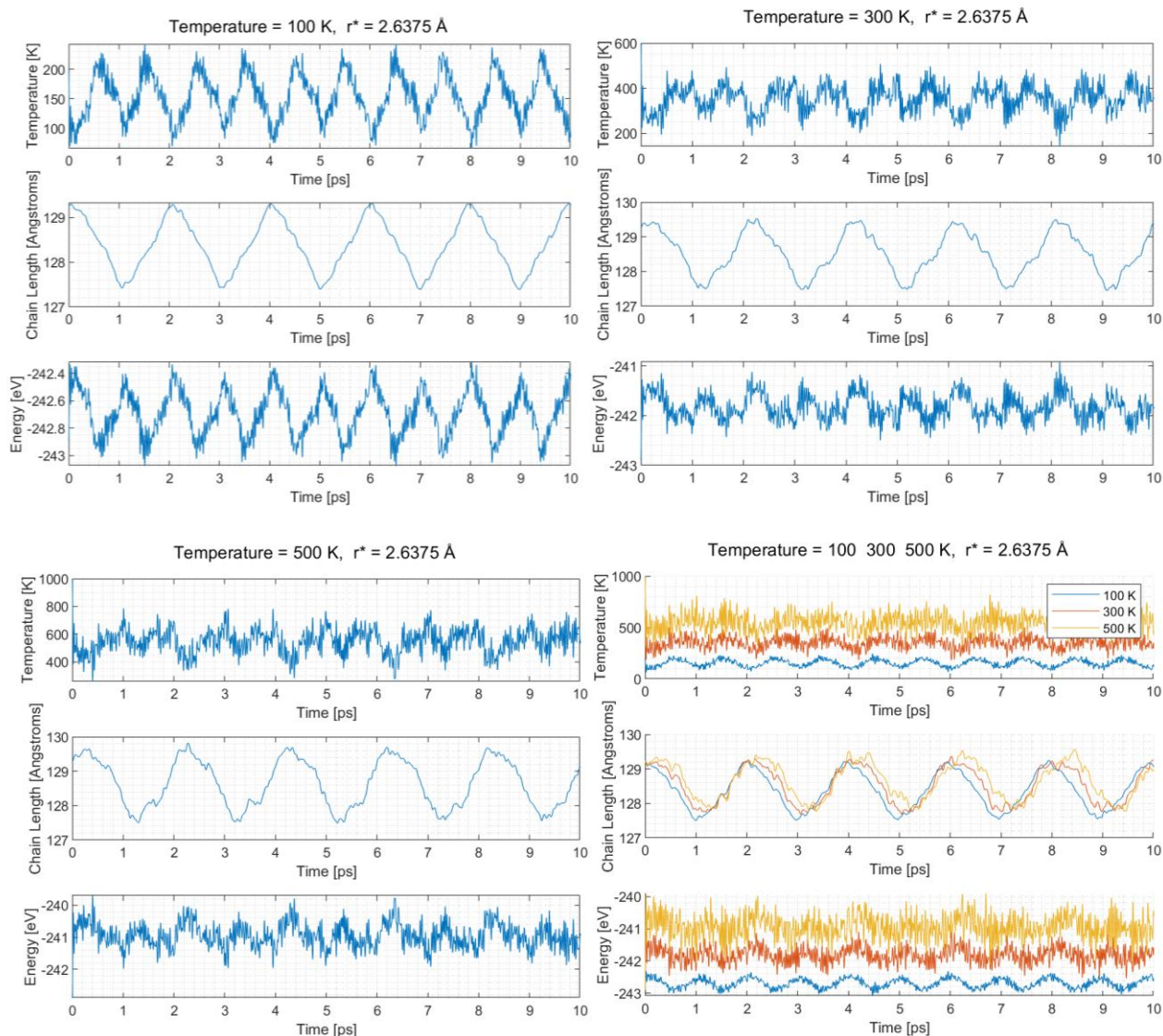


Molecular Dynamics Lab 1

1 – 4) All tests passed and completed in Matlab grader for parts 1 – 4.

5i) Below are the plots for temperature, chain length, and energy versus time for the target temperatures 100, 300, and 500 K respectively. All plots used an initial spacing of 2.6375 Å which was determined to be the equilibrium spacing in MS Lab 1. For 100 K the temperature is constantly fluctuating up and down, and the average value of about 150 K is not the desired 100 K. For 300 and 500 K the temperatures do seem to have reached the desired equilibrium temperature. No measurements should be made in the first few initial femtoseconds of each simulation because that is where the temperature steeply drops from double the target temperature. One observation with regards to the chain length is that the higher the temperature the more 'jagged' or less smooth the chain length plot appears.



5ii) Below are the plots for temperature, chain length, and energy versus time for the target temperatures 100, 300, and 500 K respectively. All plots used an initial spacing of 3.0 Å. The systems have reached equilibrium for temperature and energy at about 0.5 ps. However the chain length is growing at a continuous rate which indicates that the atoms kinetic energy has caused them to run away from each other, essentially the bonds between atoms have broken.

