Molecular dynamics 2015

Exercises 9 (not to any specific chapter): `mdmorse` : applications

1. (10p) Determine the bulk modulus

$$B = -V \frac{dP}{dV}$$

B of your Cu model. Is the excellent agreement you obtain with the experimental value of 1420 kbar surprising?

2. (10p) Test the melting of bulk Cu using the temperature and pressure controls. Simulate a block of Cu at different temperatures, using pressure control to keep the pressure at 0 kbar, and find the temperature at which the cell melts. Try to determine the melting temperature with an uncertainty less than 100 K. It is enough to estimate when the cell melts by visual inspection of the atom positions. How does the value compare with the experimental melting temperature?

Note that since the initial kinetic energy of atoms is set to twice the temperature, the cell may melt instantaneously (within 1 ps or so) before it has time to equilibrate to a given temperature. You can circumvent this by using `initialT < desiredT` and let the temperature control set the cell to the correct temperature. Report the obtained melting temperature, compare the result to experiment and comment on the difference.