Molecular dynamics 2015

Exercise 11 (not to any specific chapter): `mdmorse` : melting temperature by the interface method

1. (14 p) Determine the melting point of Morse Cu by constructing a cell which has both liquid and solid parts, and finding the temperature at which these are more or less in equilibrium. The most accurate way to determine the melting point is to estimate the speed of the movement of the liquid-solid interface as a function of temperature and determine the temperature where it crosses zero. In this case, however, visual inspection is enough.

Use temperature and pressure control the way you think is physically best motivated. When done properly, this is the best possible way to determine the melting point by direct simulation.

Hint: create the liquid and solid part in separate simulations which end at the same temperature close to the expected melting point[1]*, then merge these into a joint simulation cell which you first equilibrate a little while before starting longer simulations.*

Comment on the difference to the result you obtained in exercise 9.2. Why is the answer you obtain here more reliable than the one you obtained previously?

2. (6 p) Assume a Finnis-Sinclair type EAM model of a metal with only nearest neighbor interaction. The energy of atom i is expressed as

$$E_i = \frac{1}{2}\sum_{j\neq i}\phi(r_{ij}) - A\sqrt{n_i}, \quad n_i = \sum_{j\neq i}\rho(r_{ij}).$$

Show that it is possible to parameterize the model such that it gives BCC lattice as the equilibrium structure instead of FCC. *Hint: When only nearest neighbor interaction is included the nearest neighbor distance is the same for all structures, only the coordination varies.*

1. Note that this method should give a better value for T_m than the simple heating simulation of exercise 9.