Molecular dynamics 2015

Exercise 12 (not to any specific chapter): `mdmorse` : application to nanoclusters

Note: This is the last exercise.

1. (15 p) Spontaneous sintering of nanoclusters.

Simulate the spontaneous sintering of nanoclusters by creating two Cu spheres which are 20 Å in diameter. Rotate them by a random angle[1], and place them after that next to each other so that the minimum distance between atoms in the two is 4 Å[2]. After this simulate them for 100 ps at 600 K and cool after that slowly to 0 K. Repeat the whole process starting from picking a new random angle a few times to get a representative idea of what is going on.

Describe the behaviour of the system, and return a series of images which illustrates your description.

(The observed behaviour actually underlies the manufacturing of materials using powder sintering. See e.g H. Zhu, R. Averback, *Phil. Mag. Lett.* **73** (1996) 27).

2. (5 p) Stillinger-Weber potential for Si.

Express the energy of one silicon atom in a diamond lattice in the form given in the lecture notes (chapter 9, page 18).

1. Euler angles; see e.g. http://mathworld.wolfram.com/EulerAngles.html
2. I.e. less than the potential cut-off.