Defects and the atomic nature of matter

by Phil Hasnip

1. Introduction

In this demonstration we're going to use computer simulation to investigate the behaviour of defects in a material, as a function of temperature. The model we'll use is a simple forcefield whereby each atom feels a force due to every other atom, and the particular force we're using is the force generated by a Lennard-Jones potential.

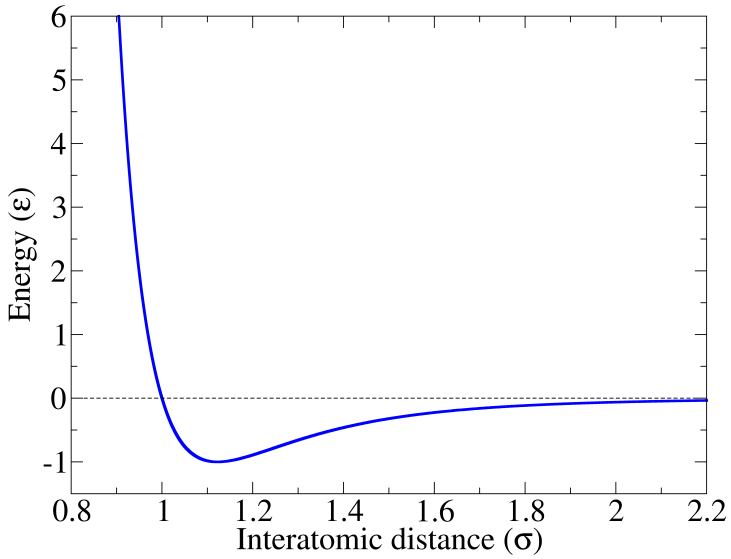
2. Lennard-Jones

The Lennard-Jones potential has two terms: an attractive, long-ranged term which decays as the sixth power of the interatomic distance; and a repulsive, short-ranged term which decays as the twelfth power of the interatomic distance.

In this model, the energy of two atoms separated by a distance r is

$$E = 4\epsilon \left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6} \right],$$

where ϵ is a parameter which controls the binding energy and σ is a parameter which controls the equilibrium interatomic distance.



The lowest energy ("ground state") of the Lennard-Jones model at low temperature is a crystal structure called *hexagonal close-packed* (hcp) though the alternative *face-centred cubic* (fcc) structure is also fairly low in energy (see for example http://www.youtube.com/watch?v=qNR2K8P-YnA).

Download the 'modelling_demo.zip', extract it and run it. You should see a chunk of a crystal, with some defects.

- How many neighbour atoms do the atoms in the main bulk of the material have?
- What defects can you see? What has caused them?

3. Atomic motion in materials

Click the 'play' button on the simulation and watch what happens.

- Is the structure stable?
- What happens as you click the blue 'cool' button a few times?
- What happens as you click the red 'heat' button a few times?

Now try clicking the red 'heat' button until the temperature is about 130 K.

- What has happened to the atomic motion?
- Where are the atoms moving most?

Investigate what happens as you slowly heat the material heat the material to around 280 K, and let the simulation run for a few moments. What happens to:

- The defects?
- Atoms near the surface?
- The bulk material?