3 TEST

COMPUTATION DETAILS

So far, we have tested this algorithm on liquid and it may be interesting to try it on crystal. Although the Fourier component of κ remains constant until q is very large, this is not the case for crystal. One of the simplest model may be the LJ crystal with fcc structure and we based our test on parameters from real crystal of Argon, so we can compare simulations with results from experiments.

We choose the crystal constant as $a = 5.31\mathring{A}$ which is $a^* = 1.56$ in LJ reduced unit (with LJ coefficient σ of Argon 3.4 $\mathring{A}$).The simulations are conducted on supoercells of $6 \times 6 \times N$ cubic conventional cells with N a parameter for approching the bulk limit. This 6 by 6 simulation proves reasonable from comparing the behaviour of $\kappa(q)$ around the $q = 0$ with that predicted by Debye Model and in order to do this, we treated the solution of Boltzmann equation in two different ways.