22.53 Problem Set II solution

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1 Problem 1

The Lennard-Jones potential is a typical two-body potential generally used in MD simulation. And it takes the form of $u(r) = 4\epsilon[(\frac{\sigma}{r})^1 2 - (\frac{\sigma}{r})^6]$, where $\epsilon\sigma$ are two parameters for certain given materials. For Argon, we have $\epsilon = 120K$ and $\sigma = 3.405A$. And, we plot the Lennard-Jone potential for Argon as figure 1.

The units of the above figure depend on what material it is. For Argon, the length unit is $\epsilon = 120K = 0.010334eV$, and the force unit is $\epsilon/\sigma = 0.010334eV/3.405A = 0.003034eV/A$. Here, we can clearly see from Figure 1 that there are mainly two parts in Lennard-Jones potential: one is the attraction part where the intermolecular distance is less than σ.The attraction part's function is to maintain the structure of the materials, which is to prevent the molecules of the material to go too far away. And the repulsive part constrains the matter to some distance away; otherwise the matter will shrink to a point due to attraction which is impossible. In fact, this potential function form agrees well with the general idea in our life. At certain temperature and pressure, a given material should have fixed density due to the balance of these two parts in potential. And, as intermolecular distance go further, the potential and force will go down approaching zero. In the figure, there exists a minumum point for the potential, which is also the mechanical balance point. It is natural to say that this the most stable state of the material at this point.

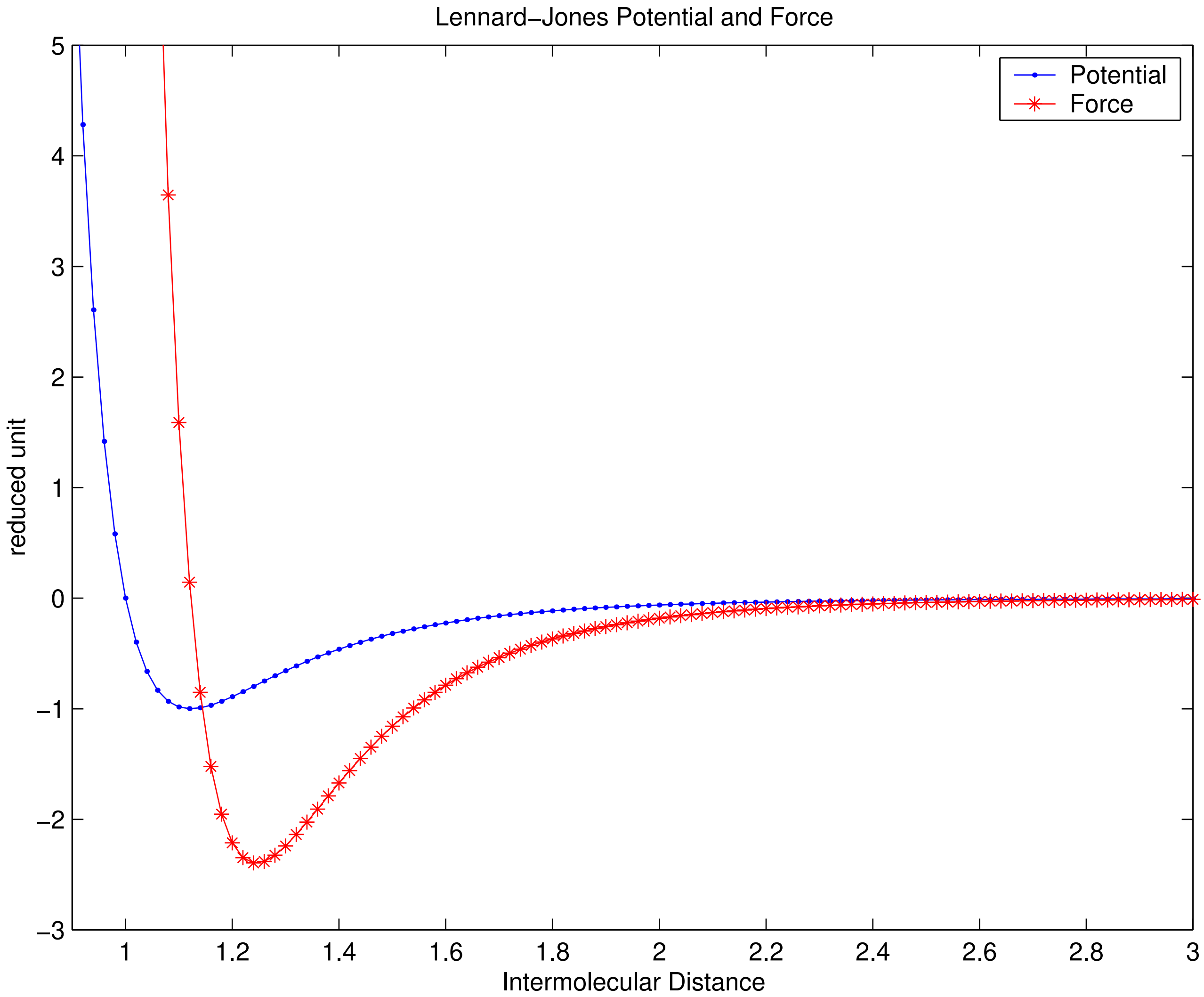

Figure 1: Lennard-Jones Potential and Its Resultant Force in Reduced Units

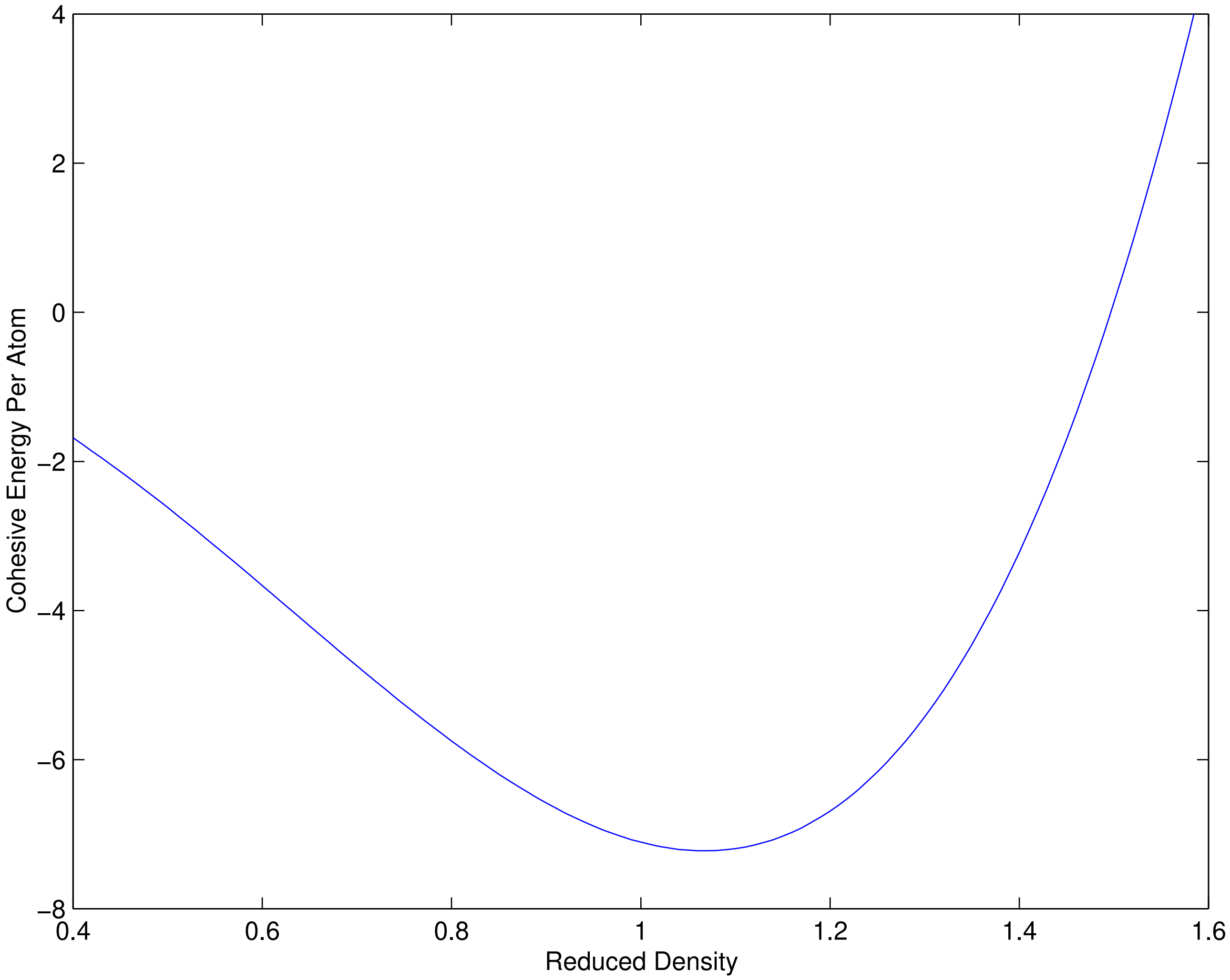

Figure 2: Reduced Cohesive energy in Face-center Cubic structure (NP=256)

2 Problem 2

First we will calculate the cohesive energy for FCC, BCC and simple cubic structures respectively. The results are shown in the following.

We can conclude from the above figures that for each structures it has its own most stable density. And onecan determine the equilibrium density (or volume) by minimizing the cohesive energy. Compared with the cohesive energy of these three structures, FCC structure is the most stable one since it has lowest cohesive energy. Furthermore, we can compare the cohesive energy per atom at a given density (or given volume) in Fig. 5 . It can be seen that

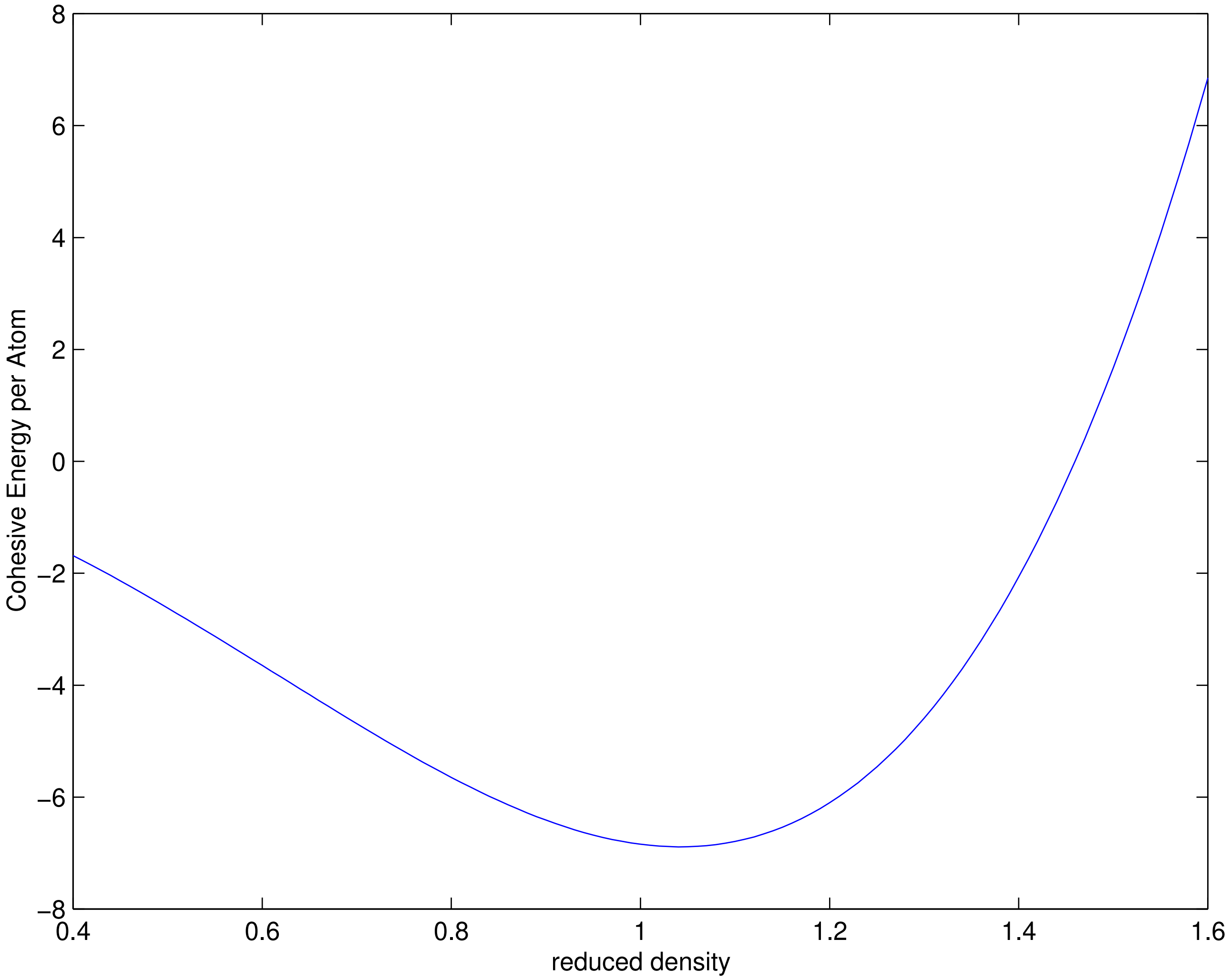

Figure 3: Reduced Cohesive energy in Body-Center Cubic structure NP=250

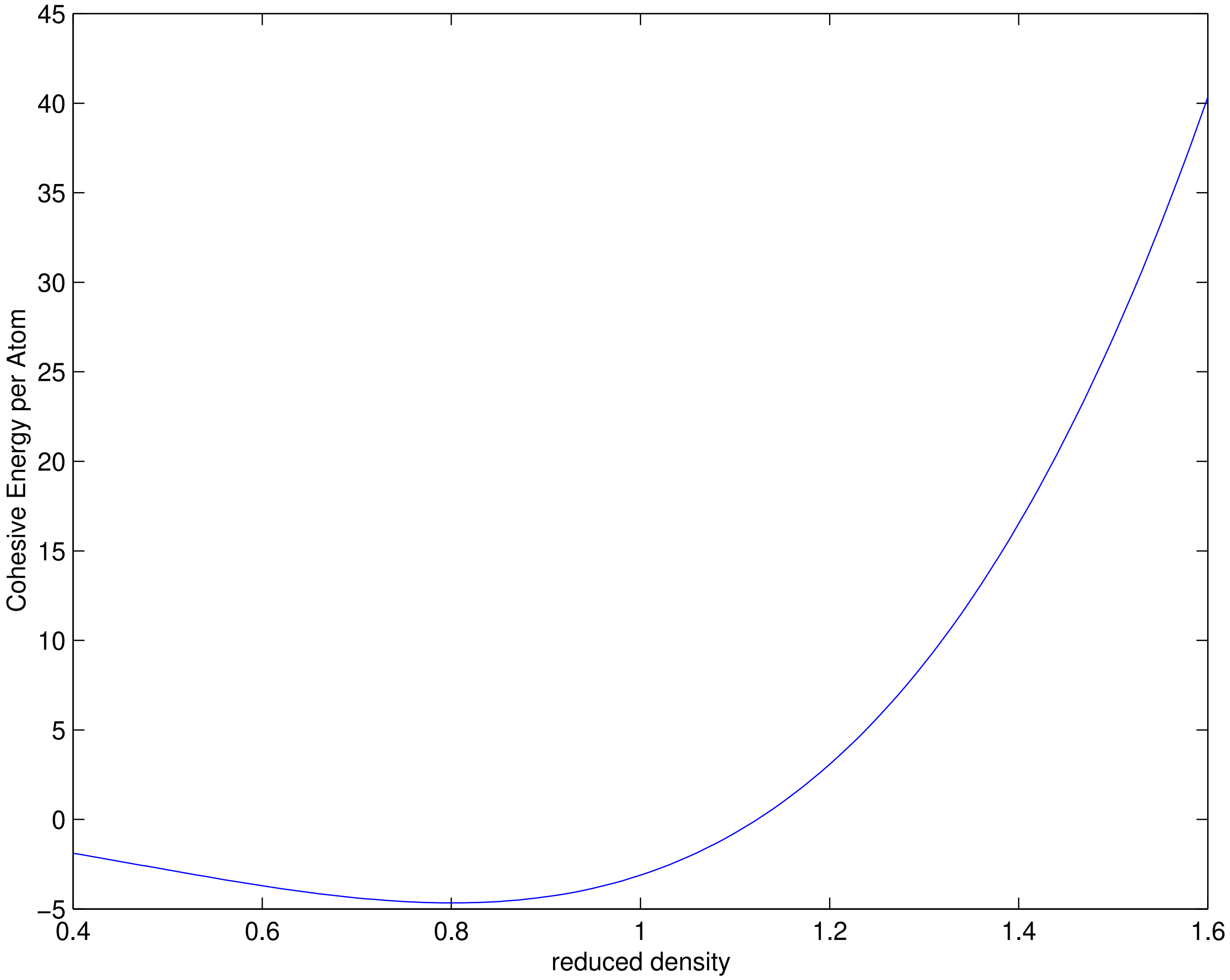

Figure 4: Reduced Cohesive energy in Simple Cubic Structure NP=216

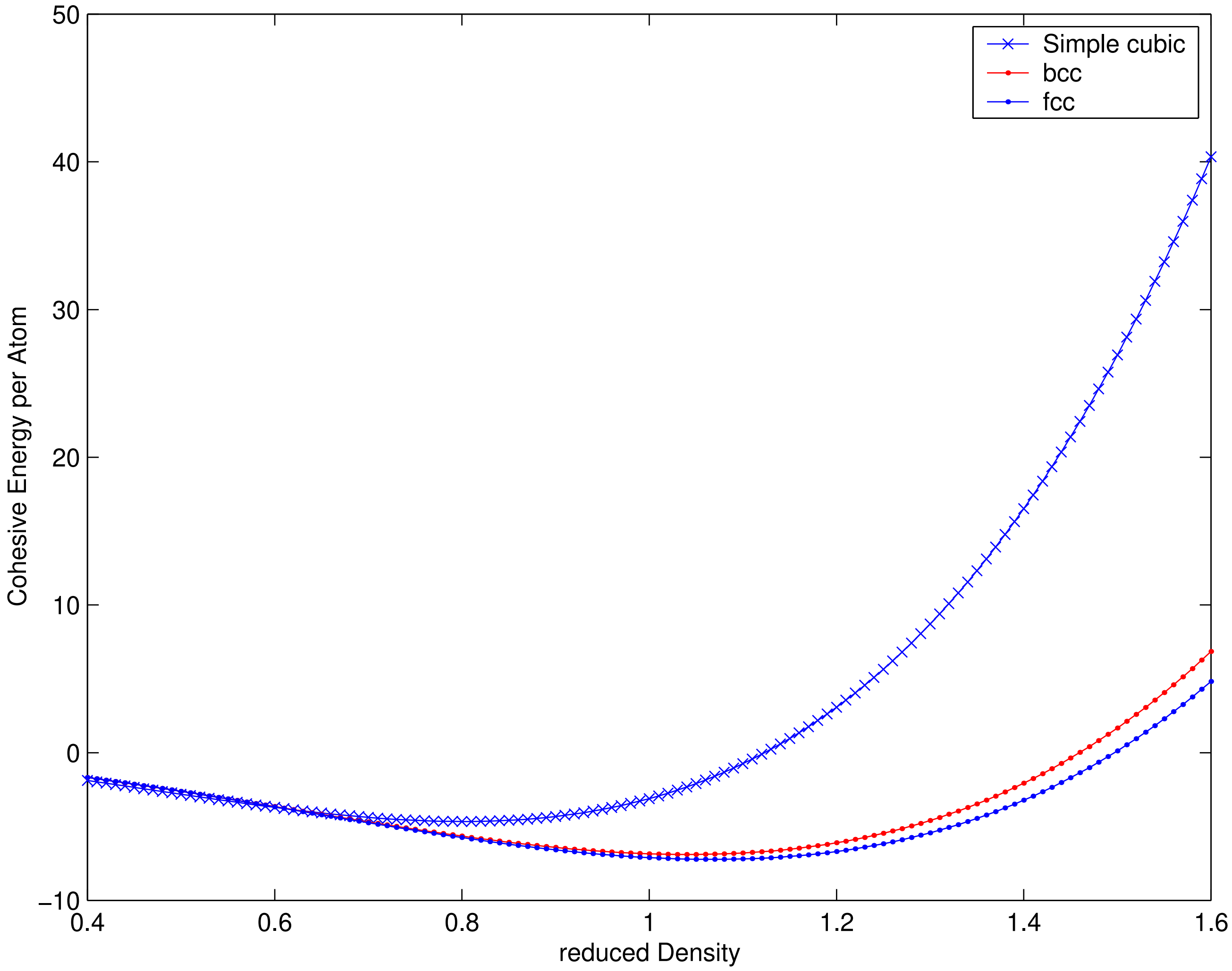

Figure 5: Compare reduced cohesive neergy in the 3 structures of FCC, BCC and simple Cupic

FCC structure is the most stable at given certain density (or volume) among these three structures.

One can image that after very long time, the high-energy state will generally go to lower energy state, and in the end, FCC structure is approached.

Next, let's calculate the presure variation with respect to density. Because the equilibrium is the minimum energy state, and it is the most stable state, we can expect that the pressure at this poin is zero. And it is indeed watched in Fig. 6.

It can be exactly examined that at equilibrium density(or volume) the pressure is zero. The

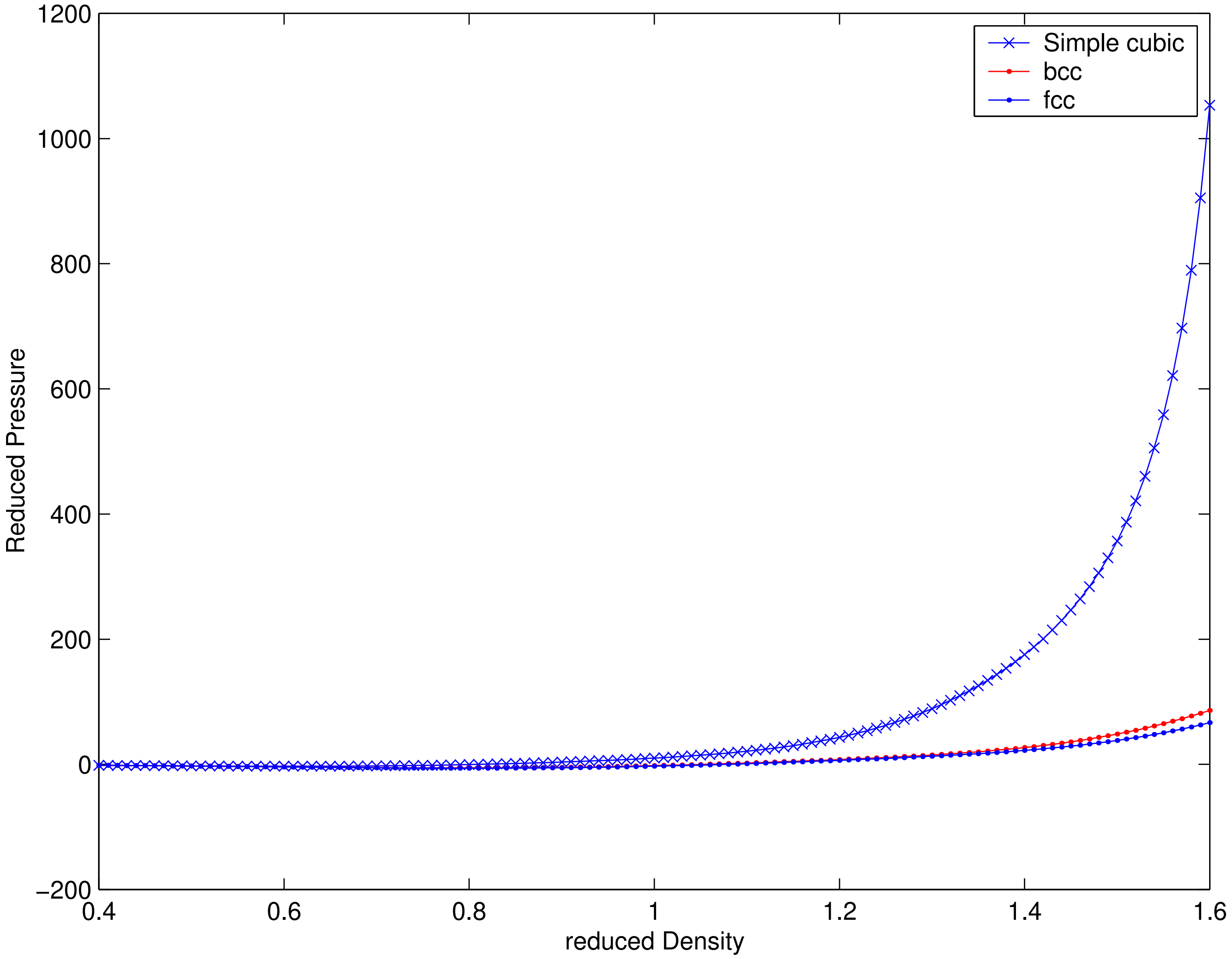

Figure 6: Reduced Pressure versus Reduced Density

table below shows cohesive energy and pressure at different equilibrium reduced densities for each structure.

Structure	Reduced Density at Equilibrium	Reduced Cohesive Energy per atom	Reduced Pressure
FCC	1.085	-8.411	0.0060
BCC	1.060	-8.048	-0.0700
Simple Cubic	0.820	-5.551	-0.0941

And it justifies our discussions. FCC structure is the favorite structure which Lennard-Jones potential will adopt. Any solid using Lennard-Jones potential must be FCC structure, and that is a restriction to the application of Lennard-Jones potential.