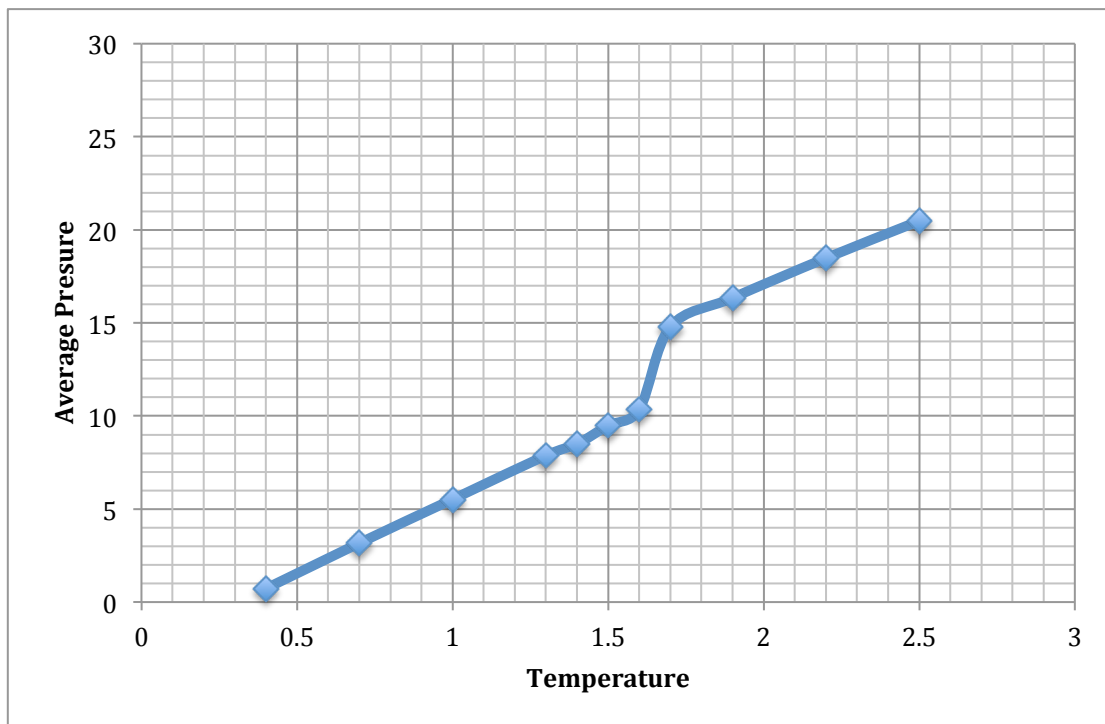12/04/2014

MD Project

I-Jou, Wang

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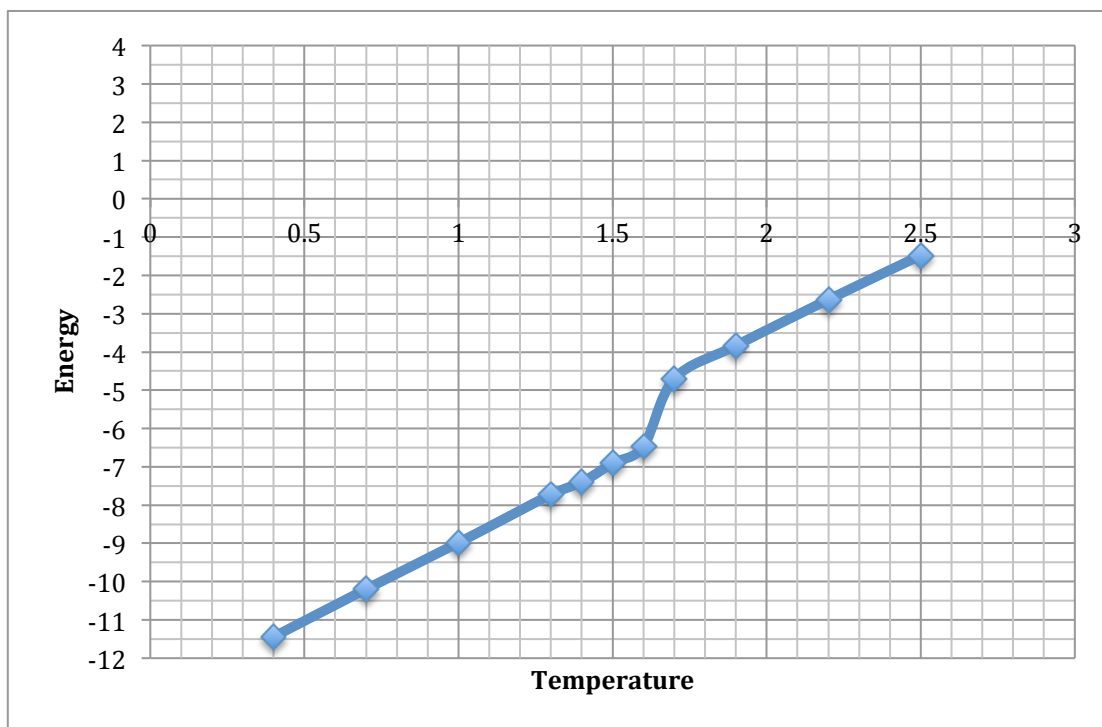ijouwang@usc.edu
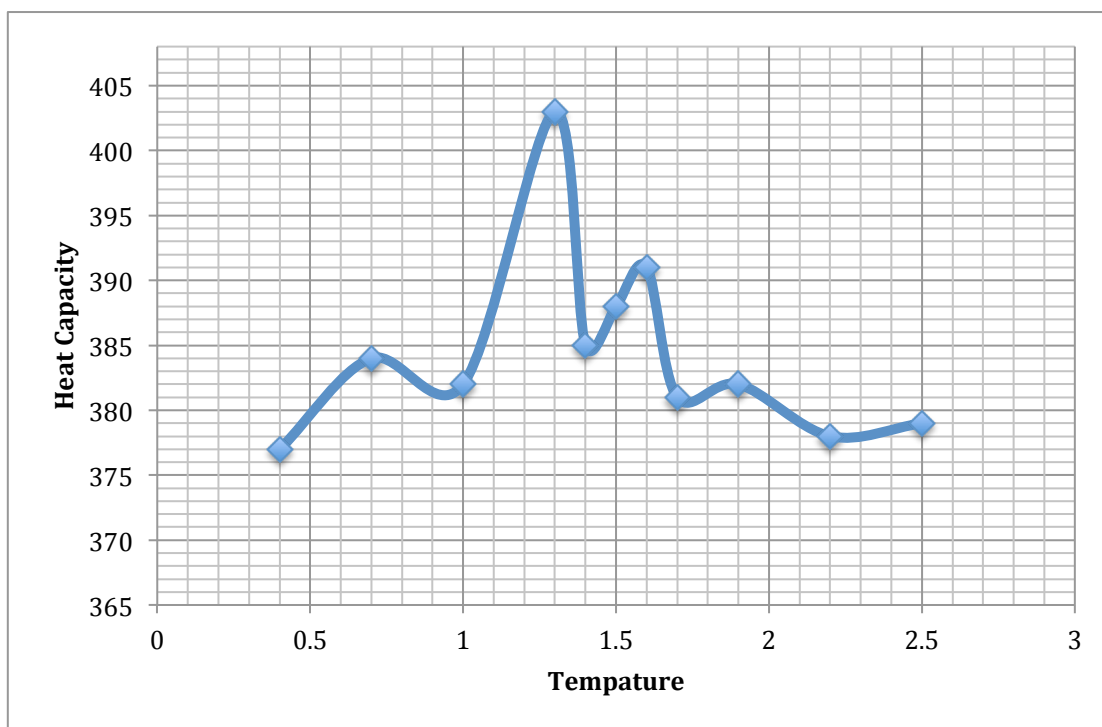
I.   Part 1

Lattice constant: 1.587401

A.   The relation between average pressure and temperature

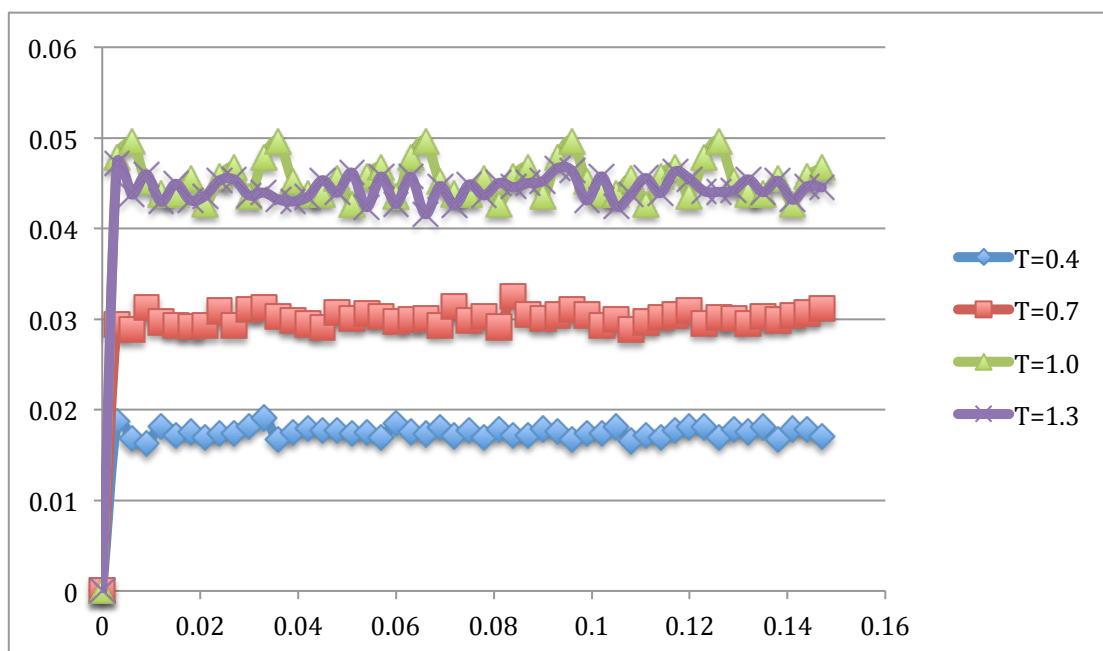## B. The relation between Energy and temperature

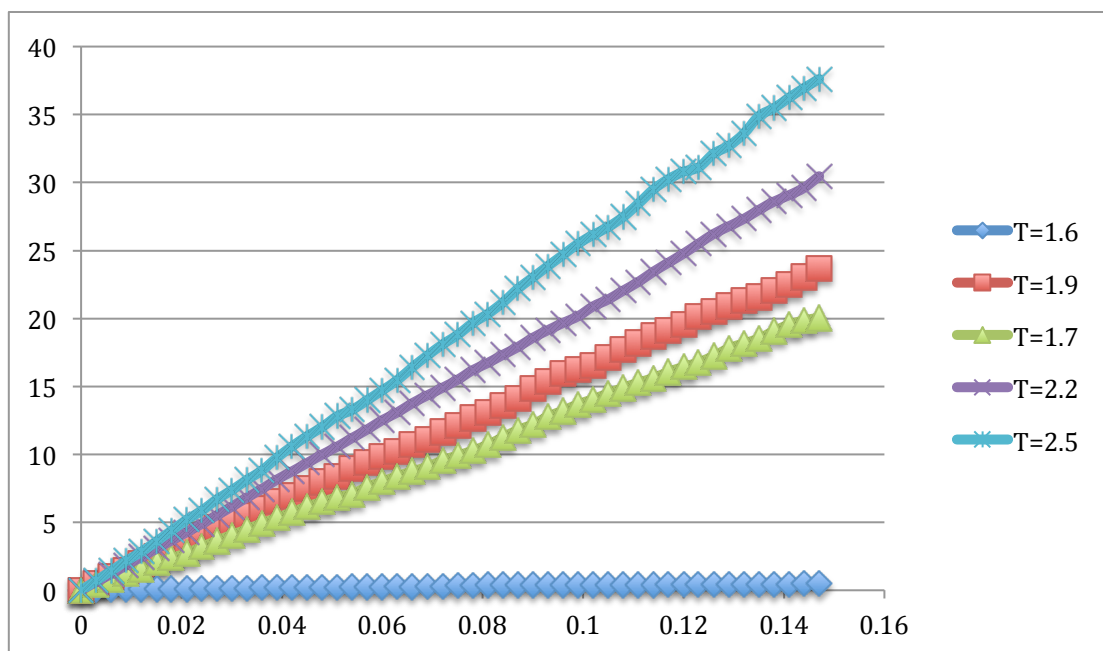## C. The relation between Energy and temperature

D.   Mean Square Displacement

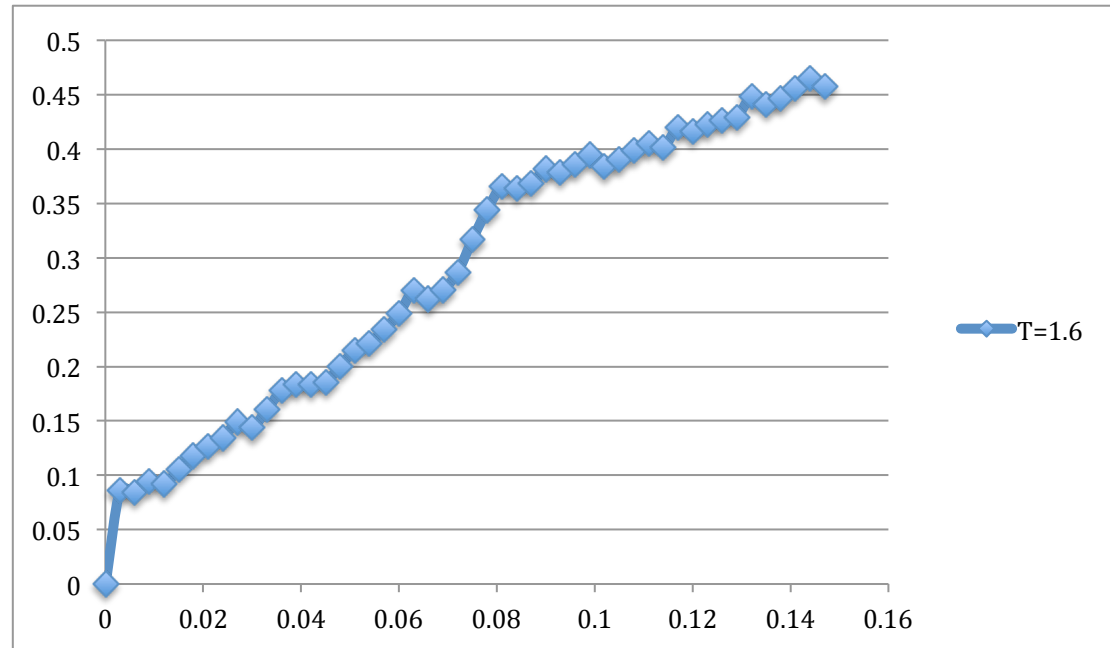**1.   Mean square displacement in solid state (below T=1.4)**

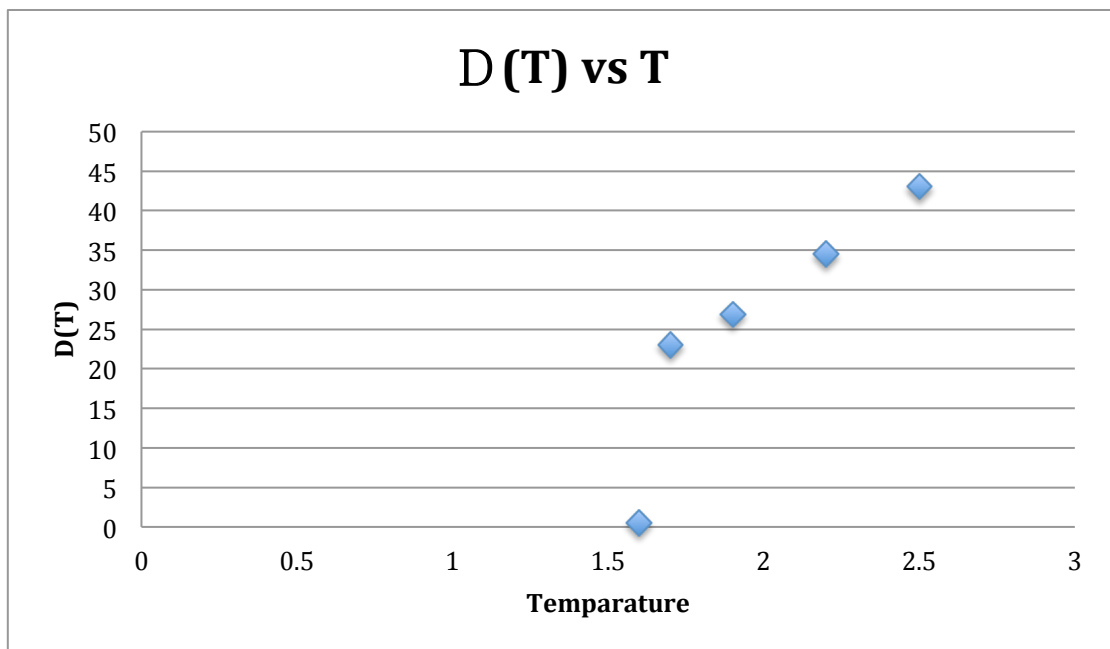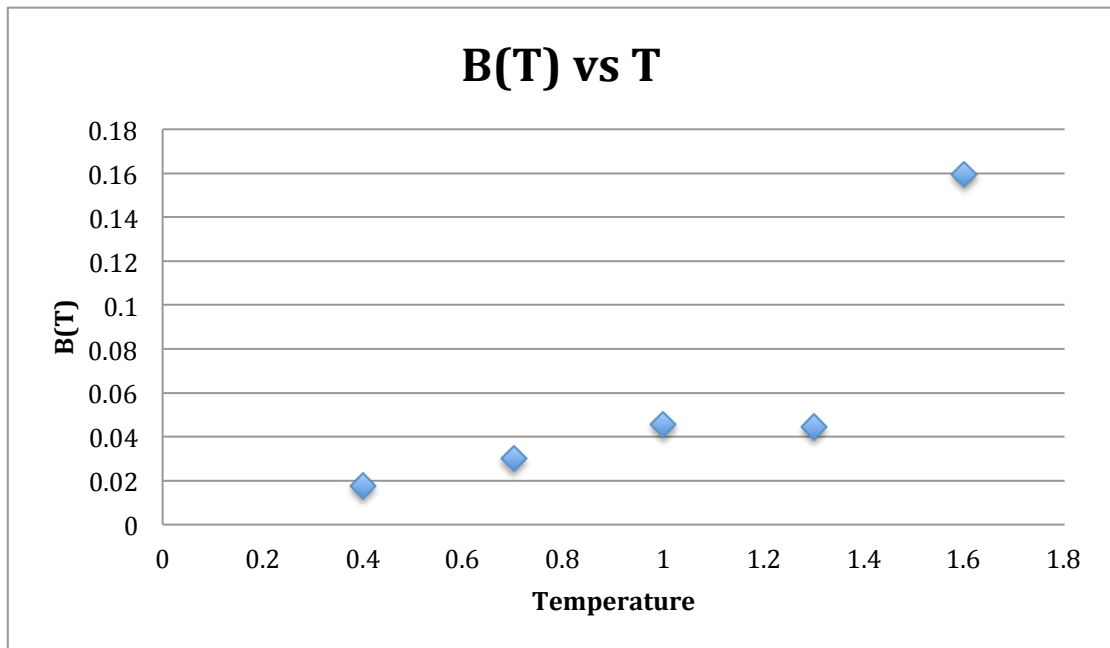**2.   Mean square displacement liquid state (above T=1.4)**

Note:

For T=1.6, the slope is not easy see in the figure above.

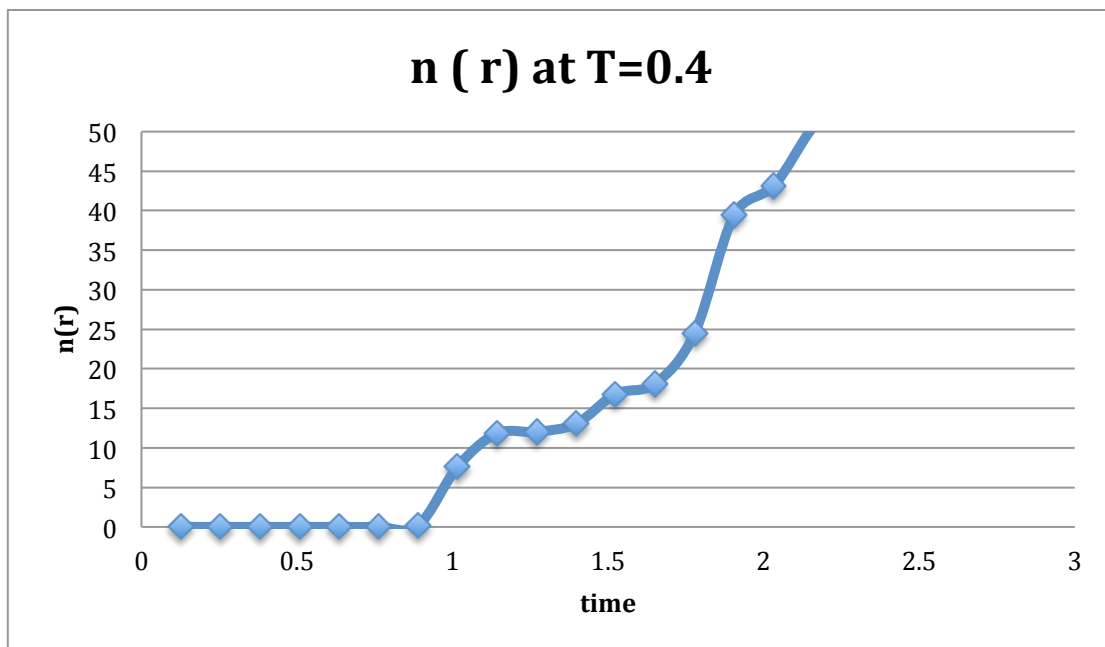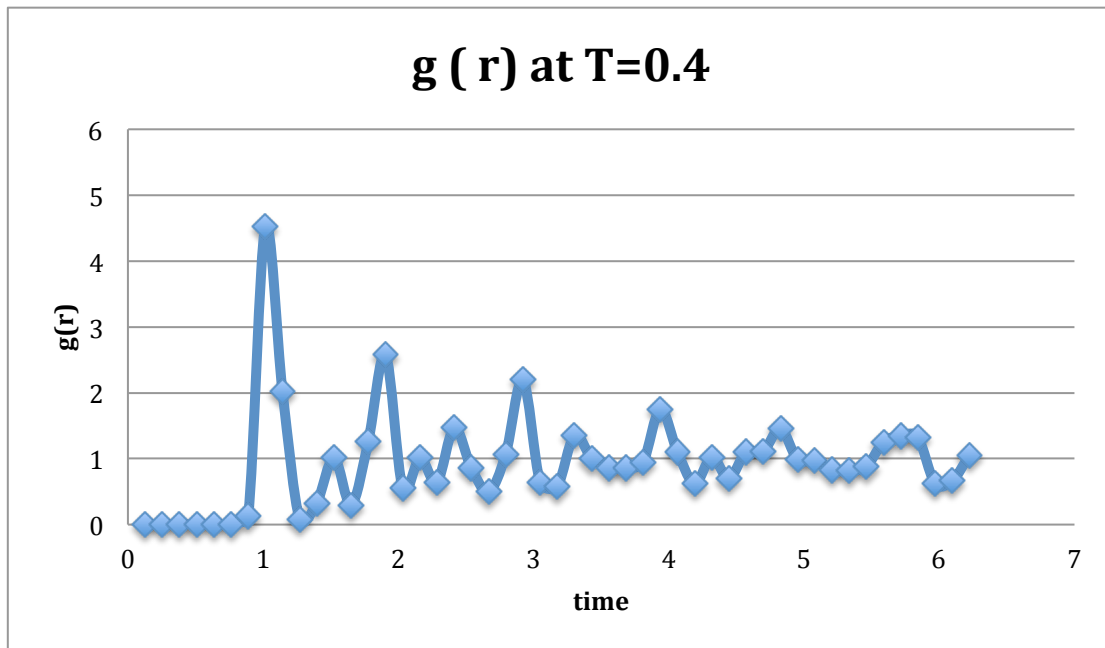According to the shape in the figure below, we can see that the state at T=1.6 is actually liquid.
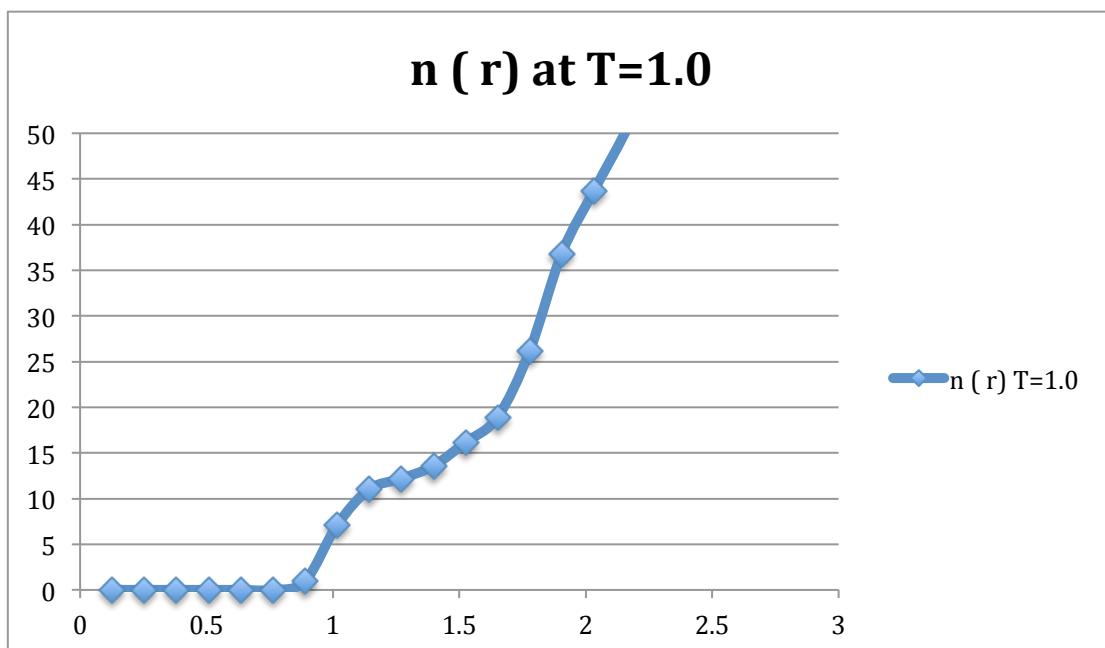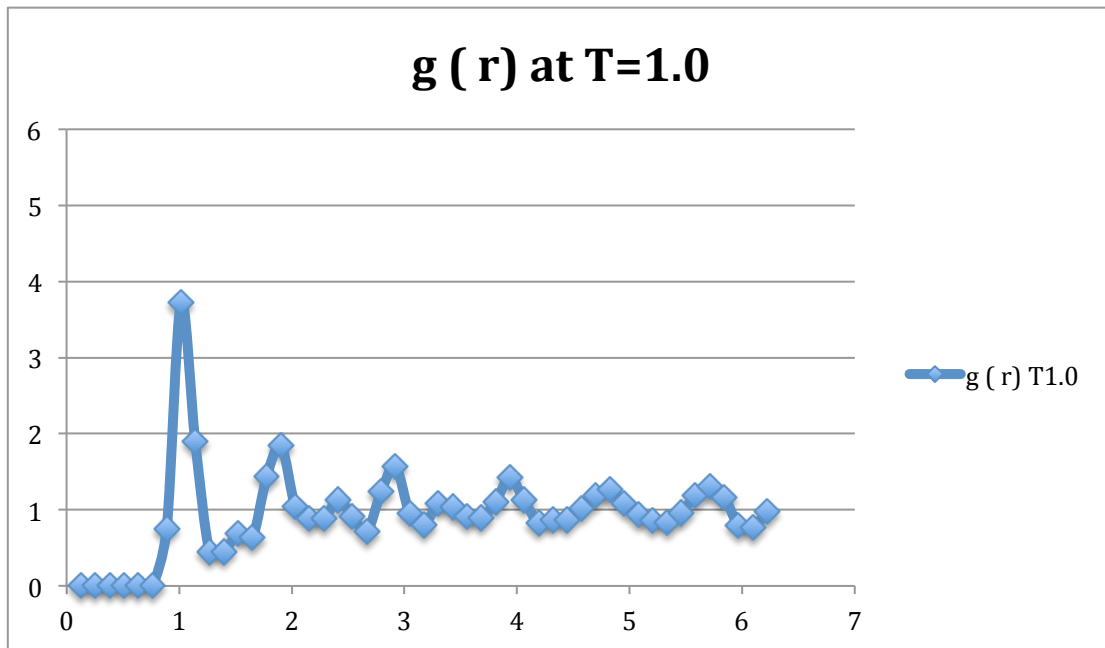
E. B(T) and D(T)

B(T) vs T

D(T) vs T

F.   g(r) and n (r)
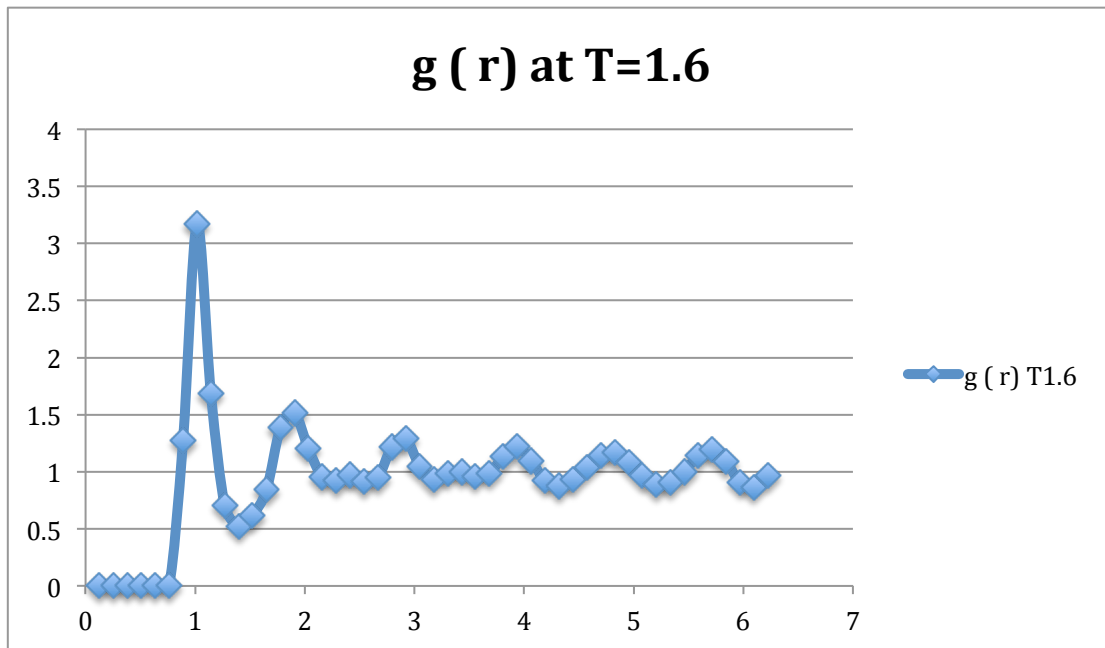
    1.   Temperature = 0.4

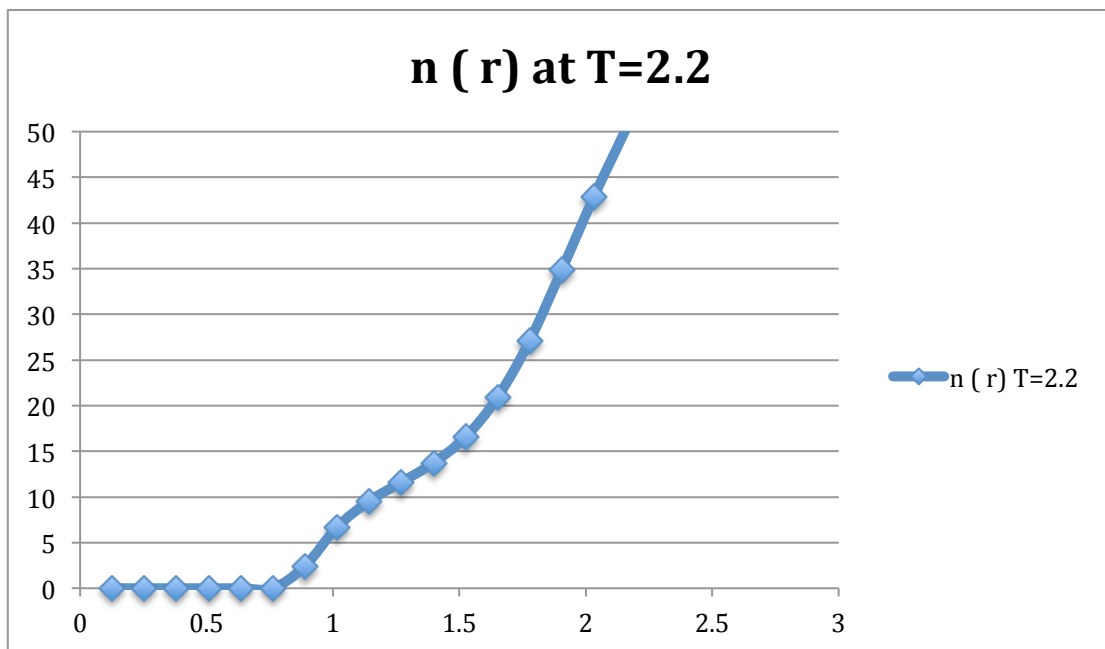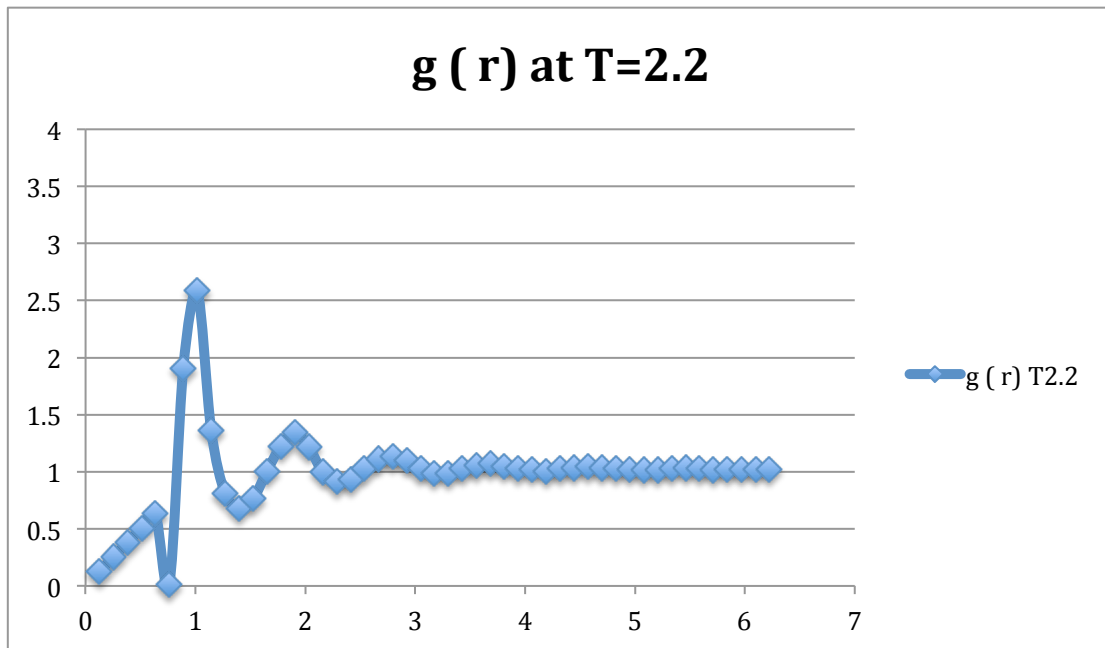**2. Temperature = 1.0**

g (r) at T=1.0

n (r) at T=1.0

3. Temperature = 1.6
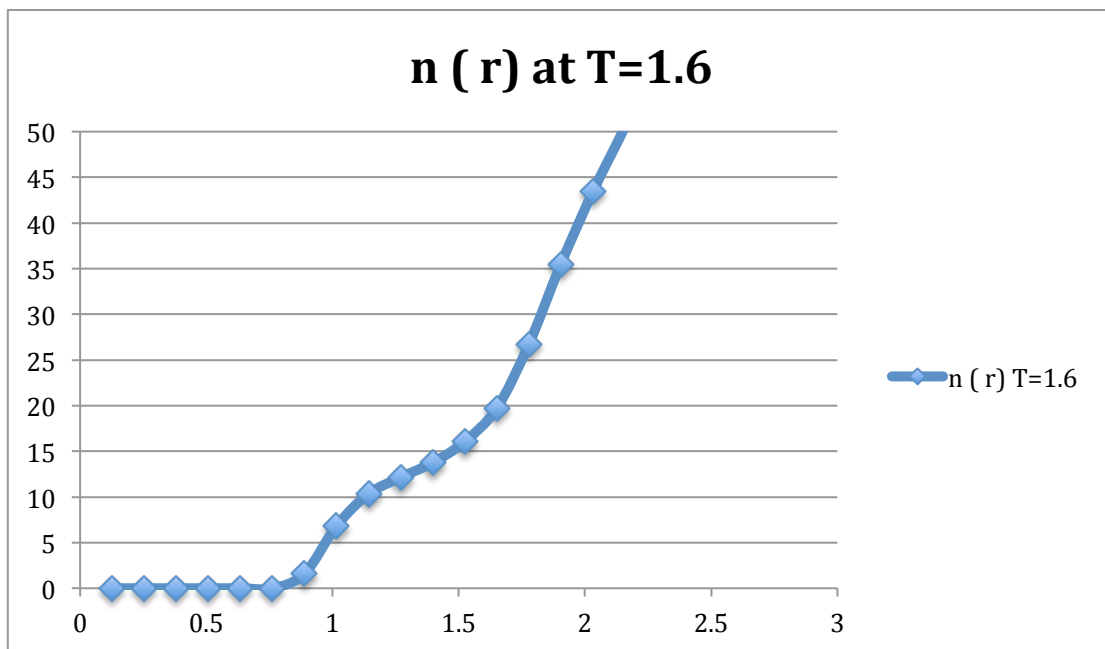
4. Temperature = 2.2
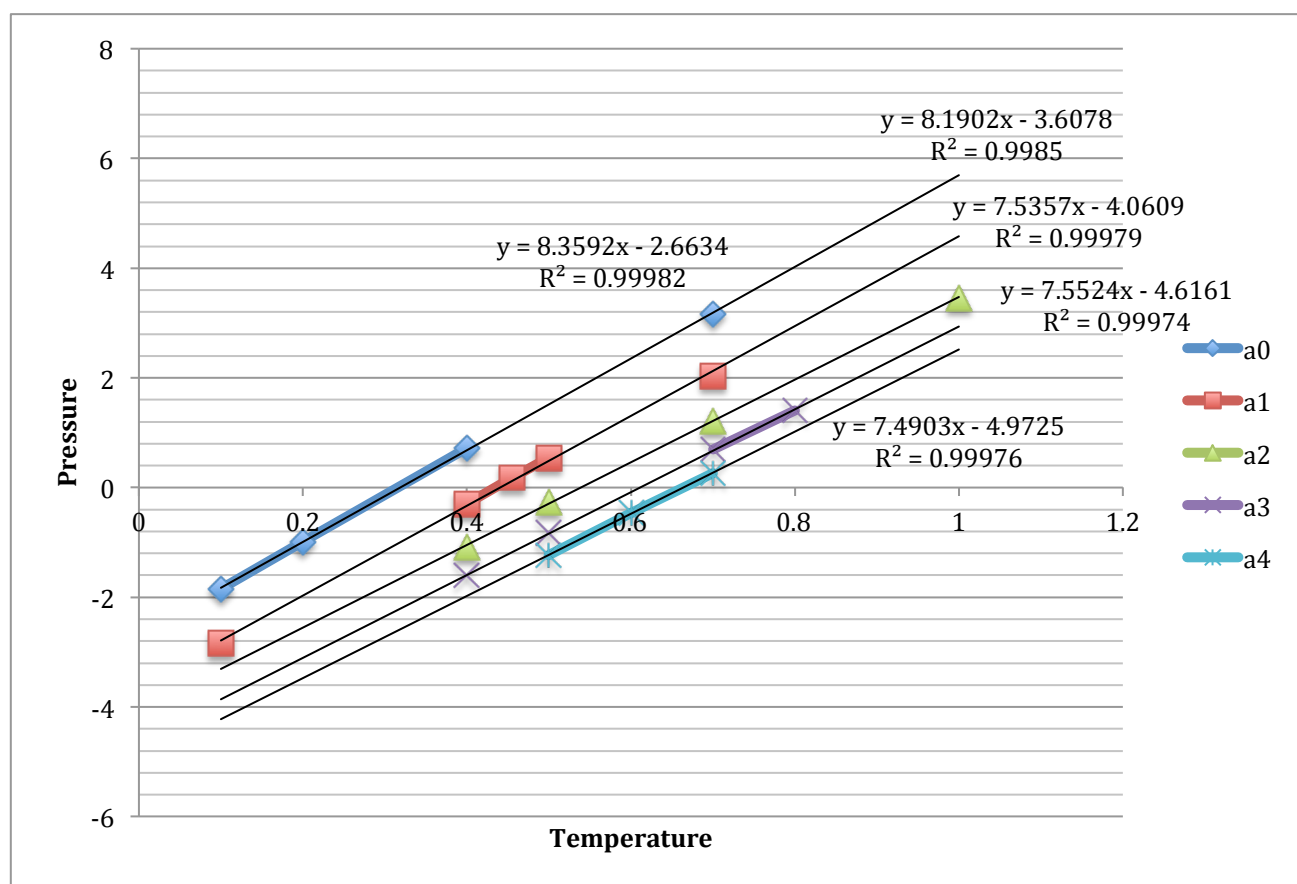
II.   Part 2

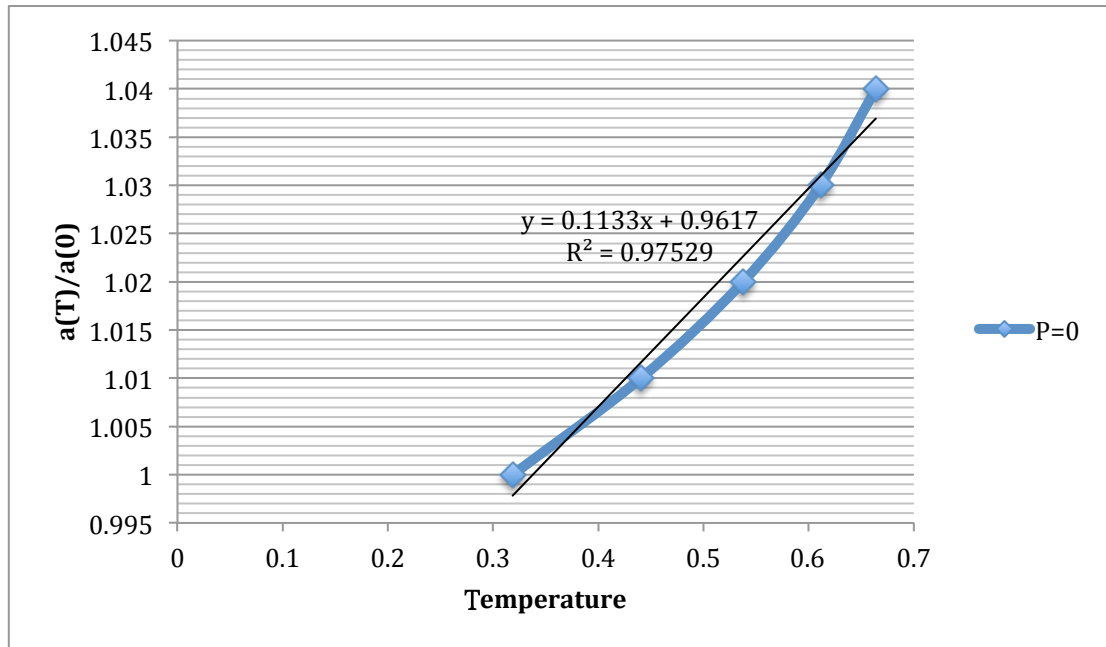### 1.   Lattice constant: 1.587401

a_1: 1.60327501

a_2: 1.61914902

a_3: 1.63502303

a_4: 1.65089704

As running the temperature close to 0.8 at a4, I found out that it is closed to melting point.

2. The slope of Temperature and a(T)/a(0) at pressure is zero

As the figure showed that the slope is 0.1133.