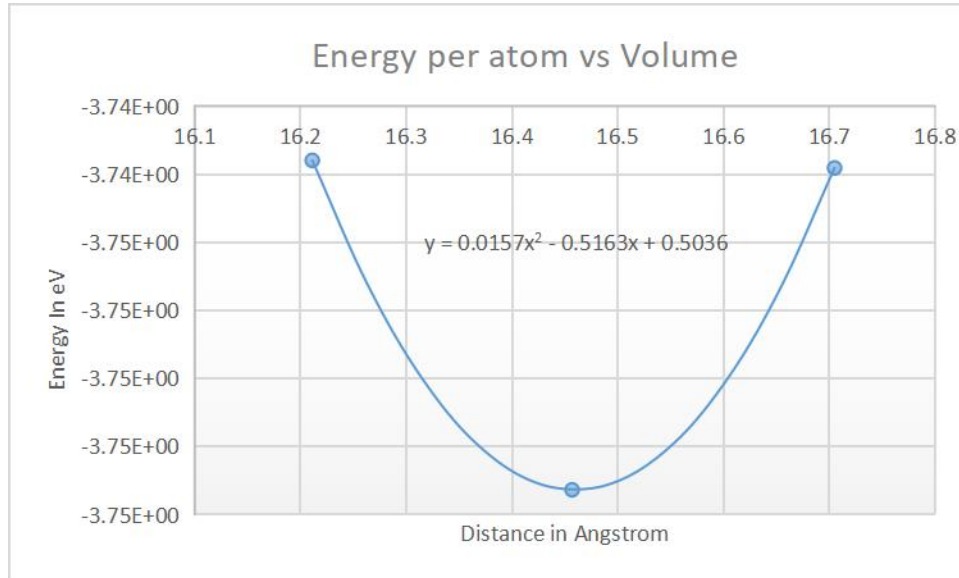


Hands On assignment 5

MM19B027 - Bhuvanesh P

1. We try to plot Energy per atom for 0.5% compression and extension of the lattice parameter. The plot is given by



2. Bulk Modulus is given by

$$B = V_0 \frac{d^2E}{dV^2}$$

$E(V)$ is given by $0.0157V^2 - 0.5163V + 0.5036$

Here V_0 is the equilibrium volume which obtained by differentiating the energy equation and equating it to 0

$$\frac{dE}{dV} = 0 = 0.0314V - 0.5163$$

Which gives V_0 as 16.44267 \AA^3

The we double differentiate the energy equation $y = 0.0157V^2 - 0.5163V + 0.5036$ to get $\frac{d^2E}{dV^2} = 0.0314$

We get $B = 0.0314 \times 16.44267 = 0.5163$ which is in eV/\AA^3

To convert it into SI units, we do $0.5163 \times \frac{1.6 \times 10^{-19}}{10^{-30}}$

We get $0.82608 \times 10^{11} \text{ Pa}$ or 82.6 GPa . Experimental value is 76 GPa . The deviation from the actual value is about 8.7% .