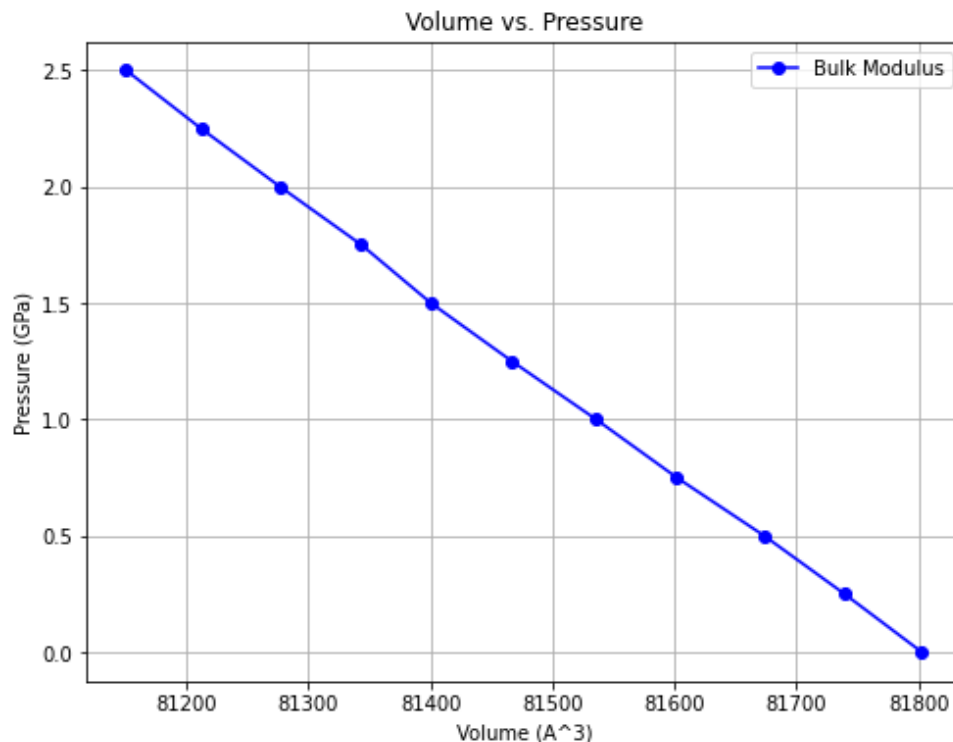Chase Katz
MSEN 470
HW4

Part 2:

Potential Comparison: SiC_1989.tersoff potential has higher error and lower R squared value when compared to the given SiC.tersoff potential.

When increasing the pressure by 0.25 GPa for each increment, the volume decreases steadily. The decrease in volume for each increase of 0.25 GPa is around 75 A^3, due to hydrostatic pressure. This is a constant linear relationship.
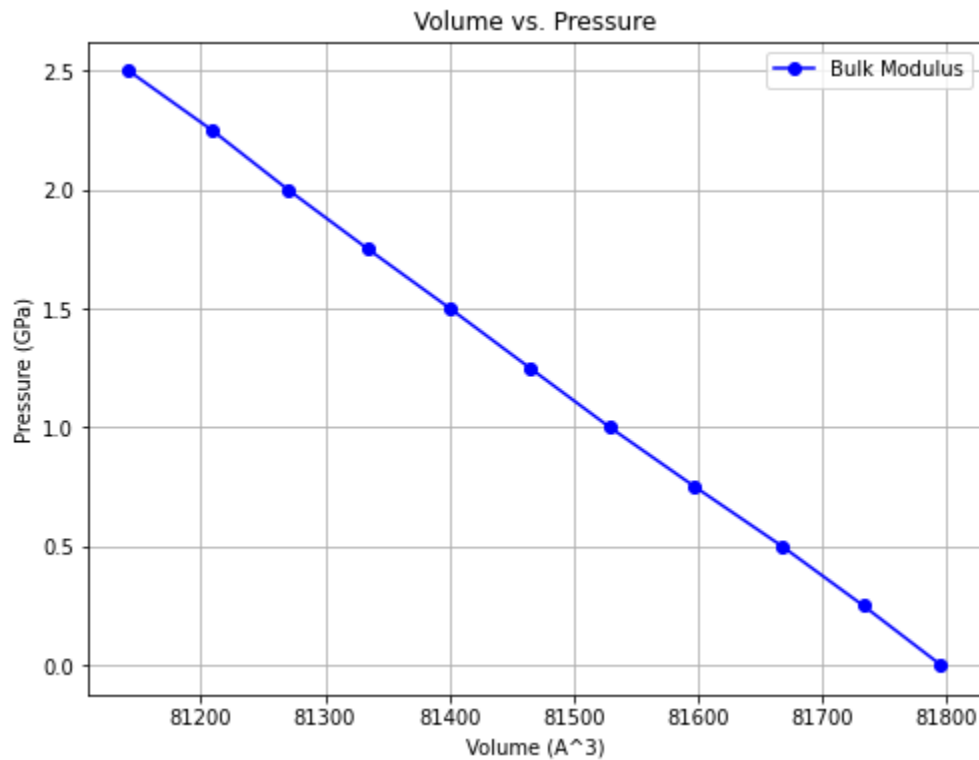
Tersoff Potential
Bulk Modulus: 313.8192141400907 GPa

Press: 0.0001 GPa	Volume: 81802.49386080066 A^3	Error:+- 48.64012277698583
Press: 0.25 GPa	Volume: 81739.1835521855 A^3	Error:+- 34.23858280110379
Press: 0.5 GPa	Volume: 81673.3805604743 A^3	Error:+- 28.537868247435966
Press: 0.75 GPa	Volume: 81601.82380579537 A^3	Error:+- 32.821750342583854
Press: 1.0 GPa	Volume: 81535.75823015194 A^3	Error:+- 32.49667448902153
Press: 1.25 GPa	Volume: 81466.79414749063 A^3	Error:+- 28.507975213372895
Press: 1.5 GPa	Volume: 81400.41289326834 A^3	Error:+- 35.95110879535124
Press: 1.75 GPa	Volume: 81343.55224132322 A^3	Error:+- 34.921279898195074
Press: 2.0 GPa	Volume: 81276.86823643501 A^3	Error:+- 28.174160512937895
Press: 2.25 GPa	Volume: 81212.16530679335 A^3	Error:+- 31.63339632569608
Press: 2.5 GPa	Volume: 81150.85098748913 A^3	Error:+- 32.03698675853467

SiC_1989.tersoff Potential

Bulk Modulus: 313.2605185505086 GPa

Volume vs. Pressure

Press: 0.0001 GPa	Volume: 81795.05795666736 A^3	Error:+- 25.687681603333917
Press: 0.25 GPa	Volume: 81732.69060780347 A^3	Error:+- 40.56373937113944
Press: 0.5 GPa	Volume: 81667.37178528408 A^3	Error:+- 31.921107780237435
Press: 0.75 GPa	Volume: 81597.34231174708 A^3	Error:+- 37.29703597527341
Press: 1.0 GPa	Volume: 81529.04610635115 A^3	Error:+- 35.25483641383997
Press: 1.25 GPa	Volume: 81464.69680119635 A^3	Error:+- 26.635393266410958
Press: 1.5 GPa	Volume: 81400.60742910656 A^3	Error:+- 34.19458346610236
Press: 1.75 GPa	Volume: 81334.65833993728 A^3	Error:+- 32.17089225635915
Press: 2.0 GPa	Volume: 81270.33439281309 A^3	Error:+- 29.594963624071124
Press: 2.25 GPa	Volume: 81209.3114003837 A^3	Error:+- 35.620385491826966
Press: 2.5 GPa	Volume: 81142.31222818544 A^3	Error:+- 32.1921039818428

Part 3:

When increasing the pressure by 0.25 GPa for each increment, the volume and strain increase steadily. The change in volume for each increase of 0.25 GPa is around 75 A^3. This is due to anisotropic pressure. The strain increases by 0.00025 for each increase of 0.25 GPa. These are steady and linear relationships.
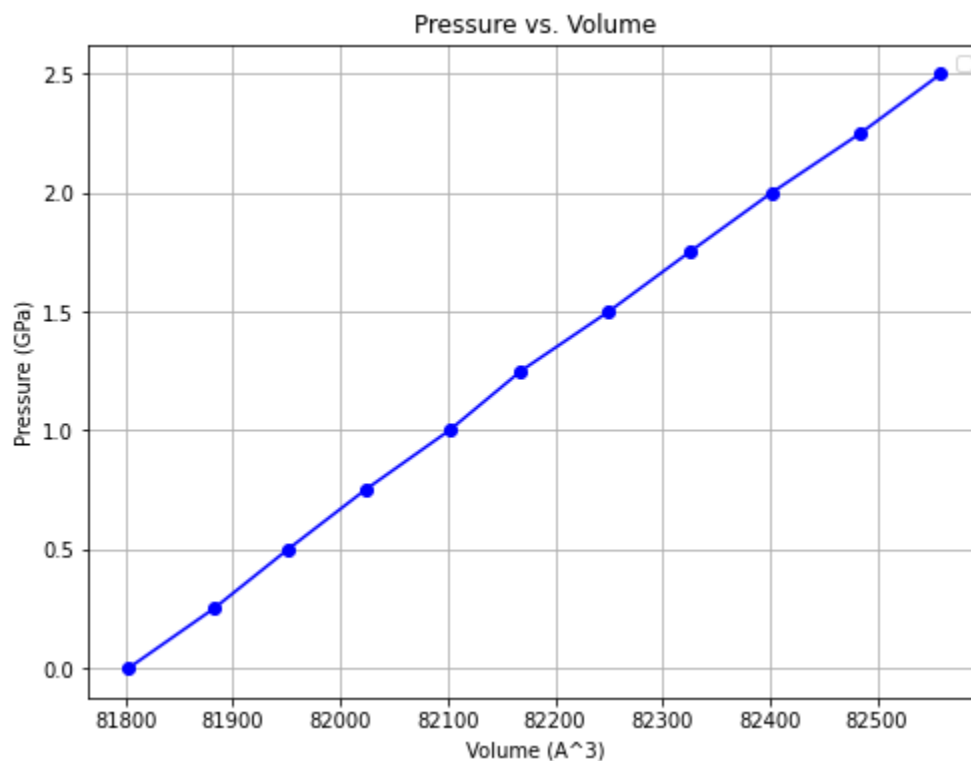
Tersoff Potential
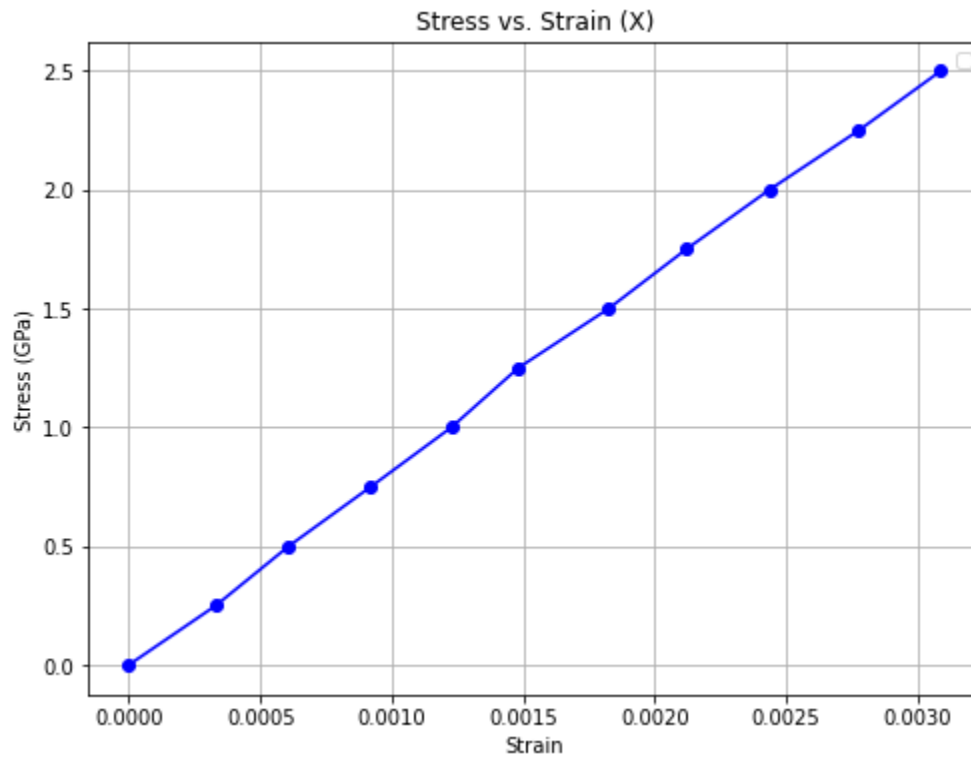Bulk Modulus: 270.5069600006339 GPa
C11: 809.8272052 GPa
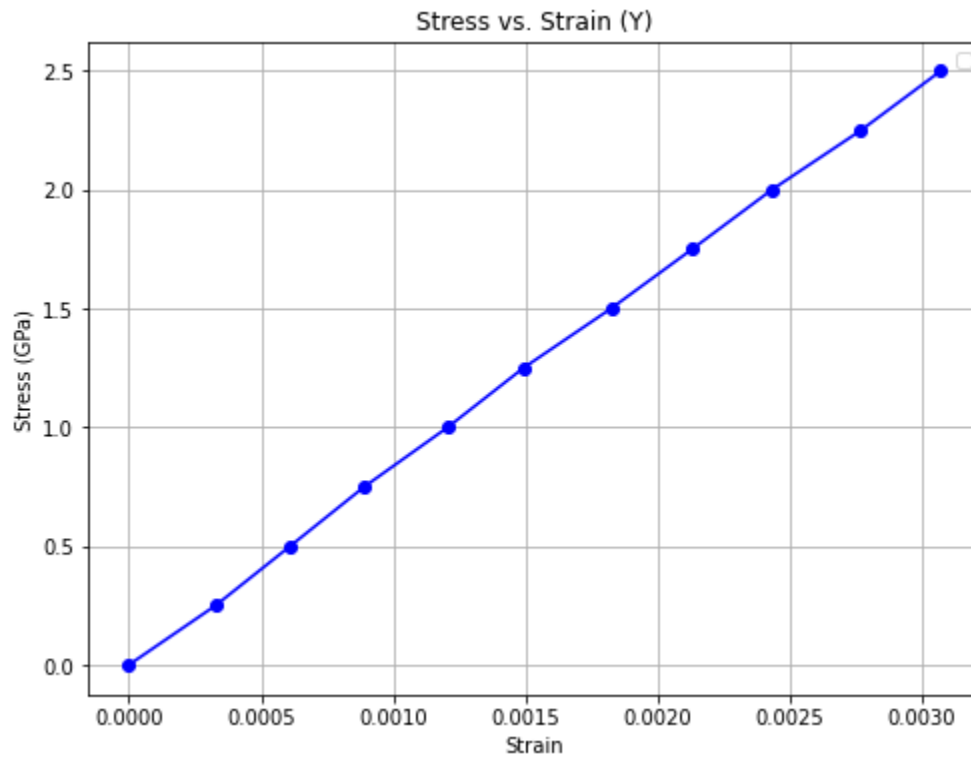C12: 814.27695146 GPa

Pressure vs. Volume

Press: 0.0001 GPa	Volume: 81803.13685592749 A^3	Error:+- 45.587815908961126
Press: 0.25 GPa	Volume: 81882.28549933893 A^3	Error:+- 32.026111948707154
Press: 0.5 GPa	Volume: 81951.52028498315 A^3	Error:+- 32.903977128761355
Press: 0.75 GPa	Volume: 82023.39760308329 A^3	Error:+- 35.56883972544132
Press: 1.0 GPa	Volume: 82101.6037755214 A^3	Error:+- 34.07531863967701
Press: 1.25 GPa	Volume: 82168.24375535619 A^3	Error:+- 46.13611502738063
Press: 1.5 GPa	Volume: 82249.90620007586 A^3	Error:+- 34.13125779174448
Press: 1.75 GPa	Volume: 82325.08069865662 A^3	Error:+- 30.022666674068407
Press: 2.0 GPa	Volume: 82401.6132358018 A^3	Error:+- 33.549125778732595
Press: 2.25 GPa	Volume: 82484.19425182491 A^3	Error:+- 44.75163227930826
Press: 2.5 GPa	Volume: 82559.123547825 A^3	Error:+- 36.082262903845745

Strain vs. Stress (X direction)

Stress vs. Strain (X)

Stress: 0.0001 GPa	Strain: 0	Error:+- 0.008688128252557789
Stress: 0.25 GPa	Strain: [0.0003308]	Error:+- 0.010321327486221972
Stress: 0.5 GPa	Strain: [0.00060811]	Error:+- 0.01226170347036084
Stress: 0.75 GPa	Strain: [0.00092005]	Error:+- 0.015611421918115272
Stress: 1.0 GPa	Strain: [0.00122649]	Error:+- 0.01154691969754788
Stress: 1.25 GPa	Strain: [0.00148084]	Error:+- 0.012055106719882934
Stress: 1.5 GPa	Strain: [0.00182451]	Error:+- 0.016531301979390574
Stress: 1.75 GPa	Strain: [0.00211992]	Error:+- 0.016344633099083135
Stress: 2.0 GPa	Strain: [0.00243562]	Error:+- 0.010265732488171767
Stress: 2.25 GPa	Strain: [0.00277562]	Error:+- 0.014968721116739326
Stress: 2.5 GPa	Strain: [0.00308695]	Error:+- 0.015090746504064218

Stress vs. Strain (Y direction)

Stress vs. Strain (Y)

Stress: 0.0001 GPa	Strain: 0	Error:+- 0.008688128252557789
Stress: 0.25 GPa	Strain: [0.00032782]	Error:+- 0.014565886048270997
Stress: 0.5 GPa	Strain: [0.00060996]	Error:+- 0.013289625025981001
Stress: 0.75 GPa	Strain: [0.00089035]	Error:+- 0.01477915390209954
Stress: 1.0 GPa	Strain: [0.00120549]	Error:+- 0.014015795814624839
Stress: 1.25 GPa	Strain: [0.00149223]	Error:+- 0.013283510696863057
Stress: 1.5 GPa	Strain: [0.0018233]	Error:+- 0.016406606377811748
Stress: 1.75 GPa	Strain: [0.00213001]	Error:+- 0.01520425831206598
Stress: 2.0 GPa	Strain: [0.00243149]	Error:+- 0.015096844762547069
Stress: 2.25 GPa	Strain: [0.00276816]	Error:+- 0.015201053413696798
Stress: 2.5 GPa	Strain: [0.00307009]	Error:+- 0.016088044162741663

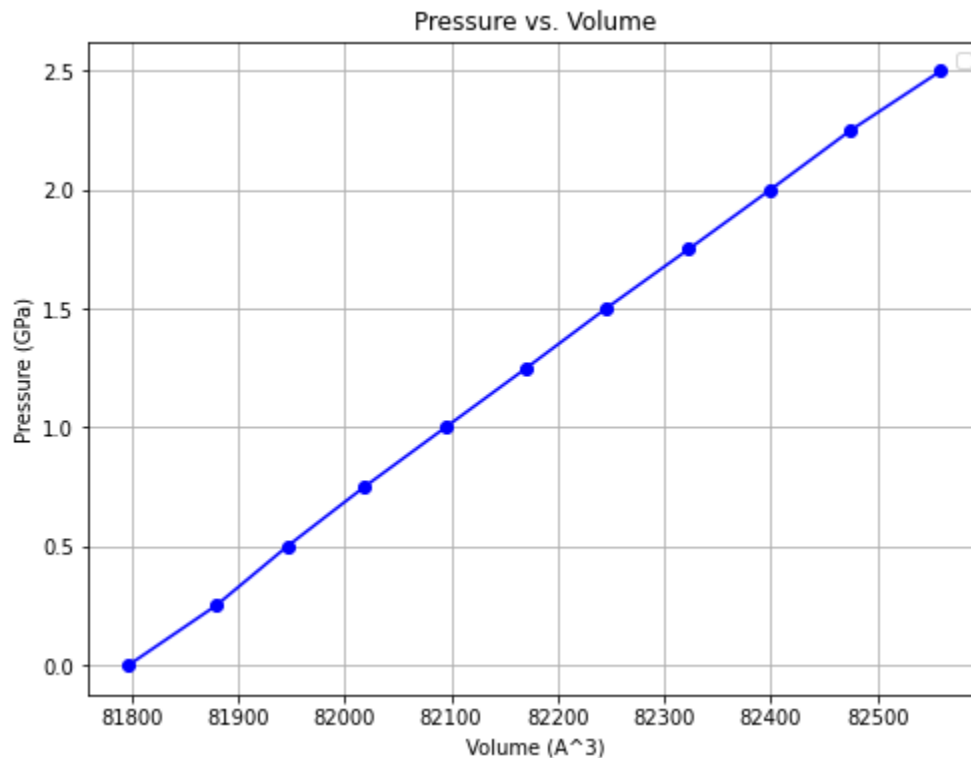# SiC_1989.tersoff Potential
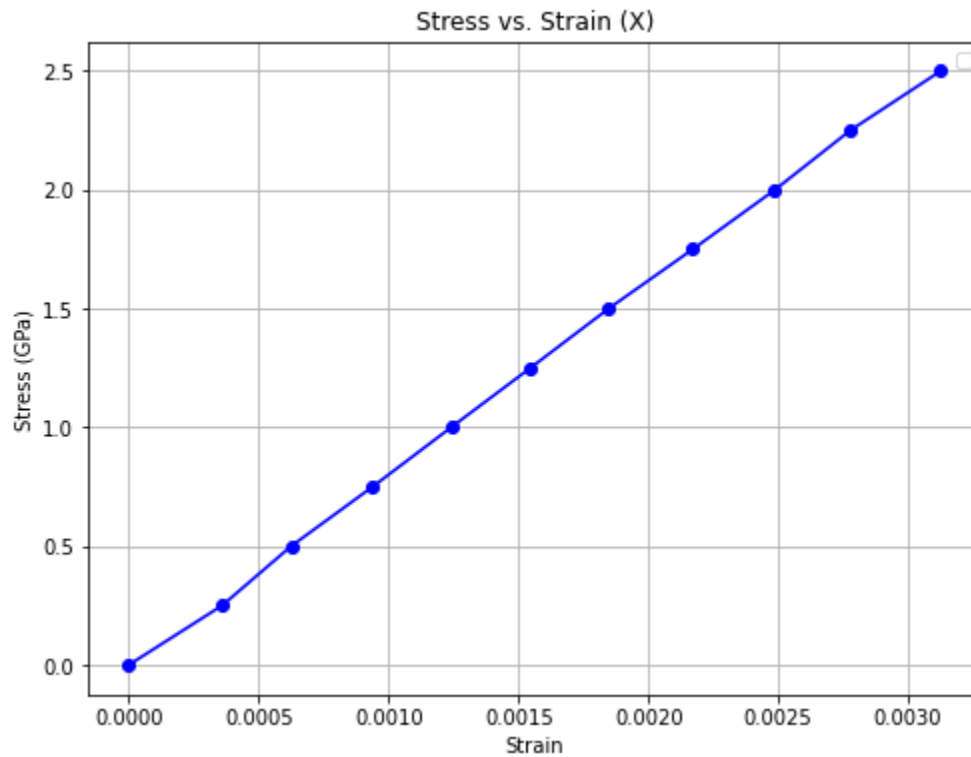Bulk Modulus: 268.39580010159426 GPa
C11: 799.95588747 GPa
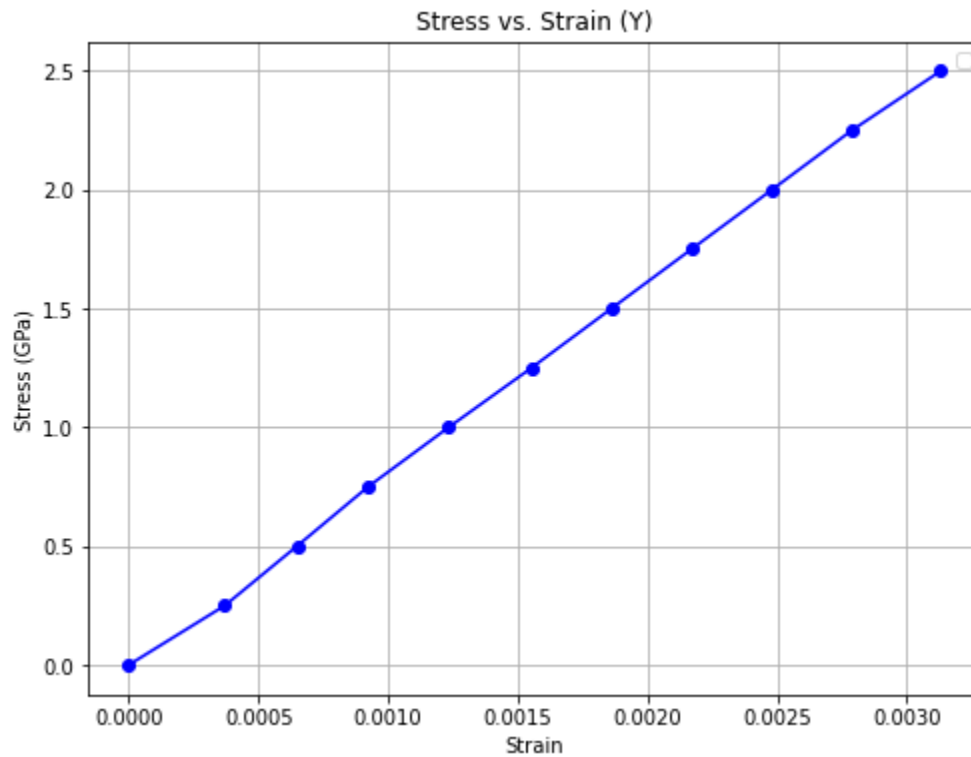C12: 798.70214531 GPa

Pressure vs. Volume

Press: 0.0001 GPa	Volume: 81797.57741713218 A^3	Error:+- 26.455505582335757
Press: 0.25 GPa	Volume: 81879.44763126115 A^3	Error:+- 33.46650437541893
Press: 0.5 GPa	Volume: 81946.44265814472 A^3	Error:+- 30.911788682849227
Press: 0.75 GPa	Volume: 82018.7385949236 A^3	Error:+- 47.008226713306286
Press: 1.0 GPa	Volume: 82094.72450216276 A^3	Error:+- 32.88466372142545
Press: 1.25 GPa	Volume: 82170.71091155255 A^3	Error:+- 32.727425729304414
Press: 1.5 GPa	Volume: 82245.26474772449 A^3	Error:+- 28.812422123755113
Press: 1.75 GPa	Volume: 82322.92546434408 A^3	Error:+- 31.545864839348887
Press: 2.0 GPa	Volume: 82399.52553068129 A^3	Error:+- 44.26774799967492
Press: 2.25 GPa	Volume: 82474.8504589487 A^3	Error:+- 33.85277315893474
Press: 2.5 GPa	Volume: 82559.45880166833 A^3	Error:+- 29.73346381483248

Strain vs. Stress (X direction)

Stress vs. Strain (X)

Stress: 0.0001 GPa	Strain: 0	Error:+- 0.011753408893765848
Stress: 0.25 GPa	Strain: [0.00035894]	Error:+- 0.014159961517063493
Stress: 0.5 GPa	Strain: [0.00062509]	Error:+- 0.016849621320918884
Stress: 0.75 GPa	Strain: [0.00093846]	Error:+- 0.013184015512073238
Stress: 1.0 GPa	Strain: [0.00124075]	Error:+- 0.011648211454729905
Stress: 1.25 GPa	Strain: [0.00154566]	Error:+- 0.012759569907090373
Stress: 1.5 GPa	Strain: [0.00184703]	Error:+- 0.01645037675730845
Stress: 1.75 GPa	Strain: [0.00217128]	Error:+- 0.01467583806456933
Stress: 2.0 GPa	Strain: [0.00248705]	Error:+- 0.012040160801552471
Stress: 2.25 GPa	Strain: [0.00277729]	Error:+- 0.013622442346979853
Stress: 2.5 GPa	Strain: [0.00312505]	Error:+- 0.013295978255429103

Stress vs. Strain (Y direction)

Stress: 0.0001 GPa	Strain: 0	Error:+- 0.011753408893765848
Stress: 0.25 GPa	Strain: [0.00037018]	Error:+- 0.014595427695686688
Stress: 0.5 GPa	Strain: [0.00064809]	Error:+- 0.013228659927373723
Stress: 0.75 GPa	Strain: [0.00092239]	Error:+- 0.011741904454972947
Stress: 1.0 GPa	Strain: [0.00123289]	Error:+- 0.016971923589573064
Stress: 1.25 GPa	Strain: [0.0015518]	Error:+- 0.01869397270970425
Stress: 1.5 GPa	Strain: [0.00186035]	Error:+- 0.0183170548397874
Stress: 1.75 GPa	Strain: [0.00216926]	Error:+- 0.016834929395726676
Stress: 2.0 GPa	Strain: [0.00247912]	Error:+- 0.015080767171772237
Stress: 2.25 GPa	Strain: [0.0027873]	Error:+- 0.013867279573081558
Stress: 2.5 GPa	Strain: [0.00312995]	Error:+- 0.012333157010781129