Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


# Nanomechanics of Antimonene Allotropes Under Tensile Loading†

Tanmay Sarkar Akash, [a] Rafsan A.S.I. Subad [a,b], Pritom Bose [a], and Md Mahbubul Islam *[c]

[a]Department of Mechanical Engineering, Bangladesh University of Engineering and Technology, Dhaka-1000, Bangladesh

[b]Department of Mechanical Engineering, University of Massachusetts Dartmouth, 285 Old Westport Road, Dartmouth, MA- 02747, USA

[c]Department of Mechanical Engineering, Wayne State University, 5050 Anthony Wayne Drive, Detroit, MI- 48202, USA

*E-mail: mahbub.islam@wayne.edu

## Supplementary Figures

For the current SW potential parameters, we found a negative out of plane Poisson's ratio at strain larger than 15% (Figure S1).

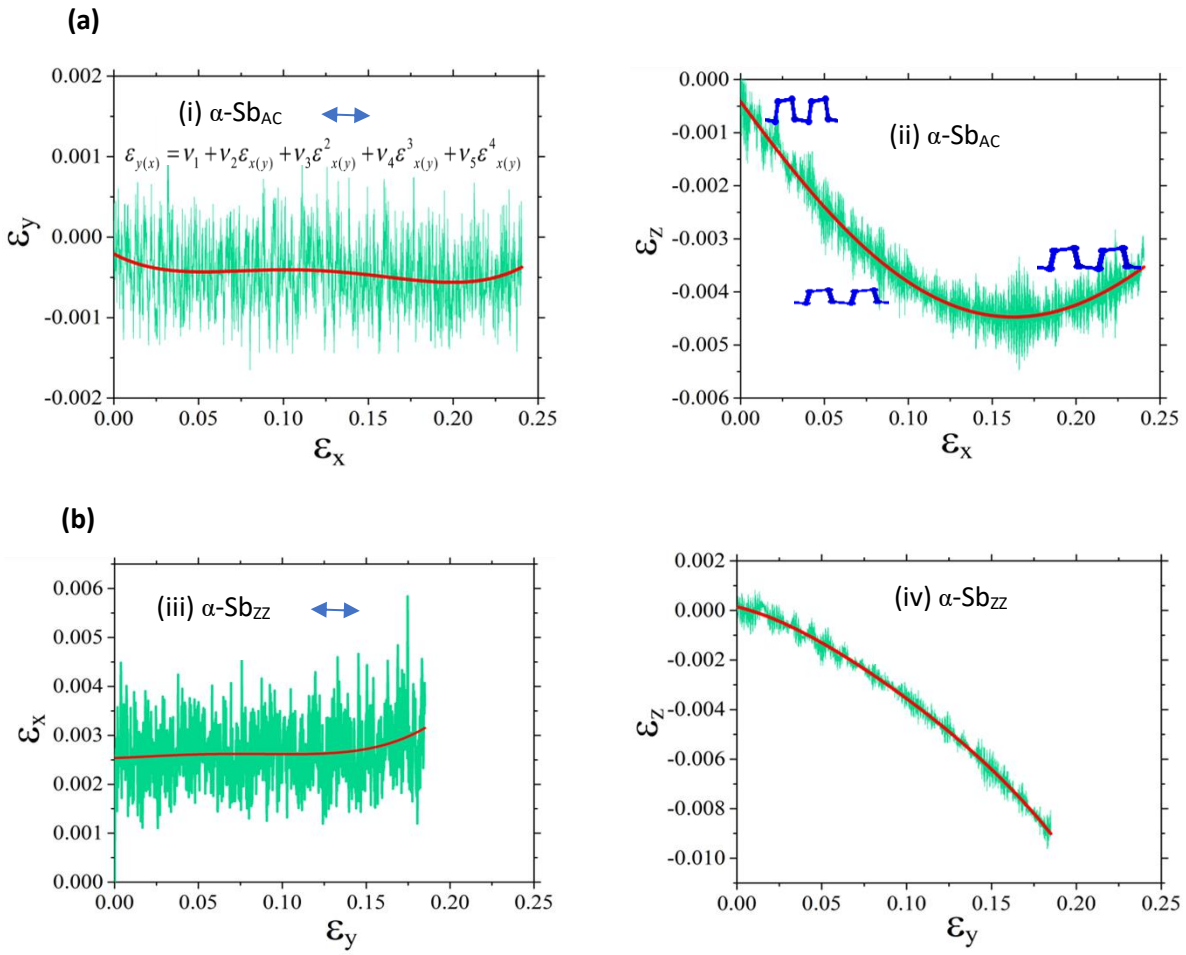



**Figure S1: Strain responses of α-antimonene to the non-loading axes for (a) armchair loading and (b) zigzag loading**

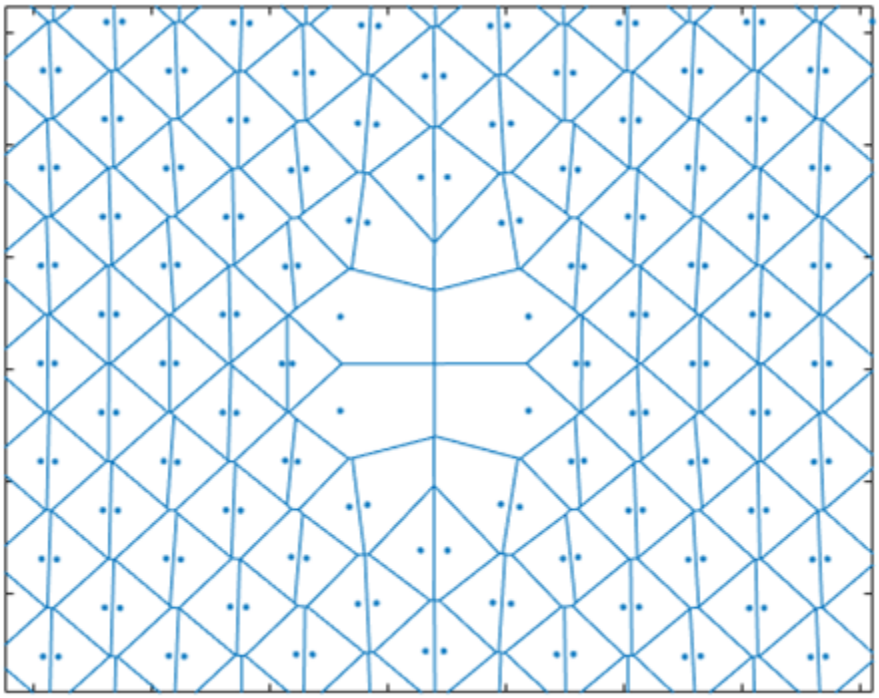


**Figure S2: Voronoi areas for atoms in a cracked α-antimonene sample. Volumes are calculated with a uniform thickness of 1 nm. Note that, volumes of crack edge atoms (except crack-tips) are ill-defined and not used in our calculations**

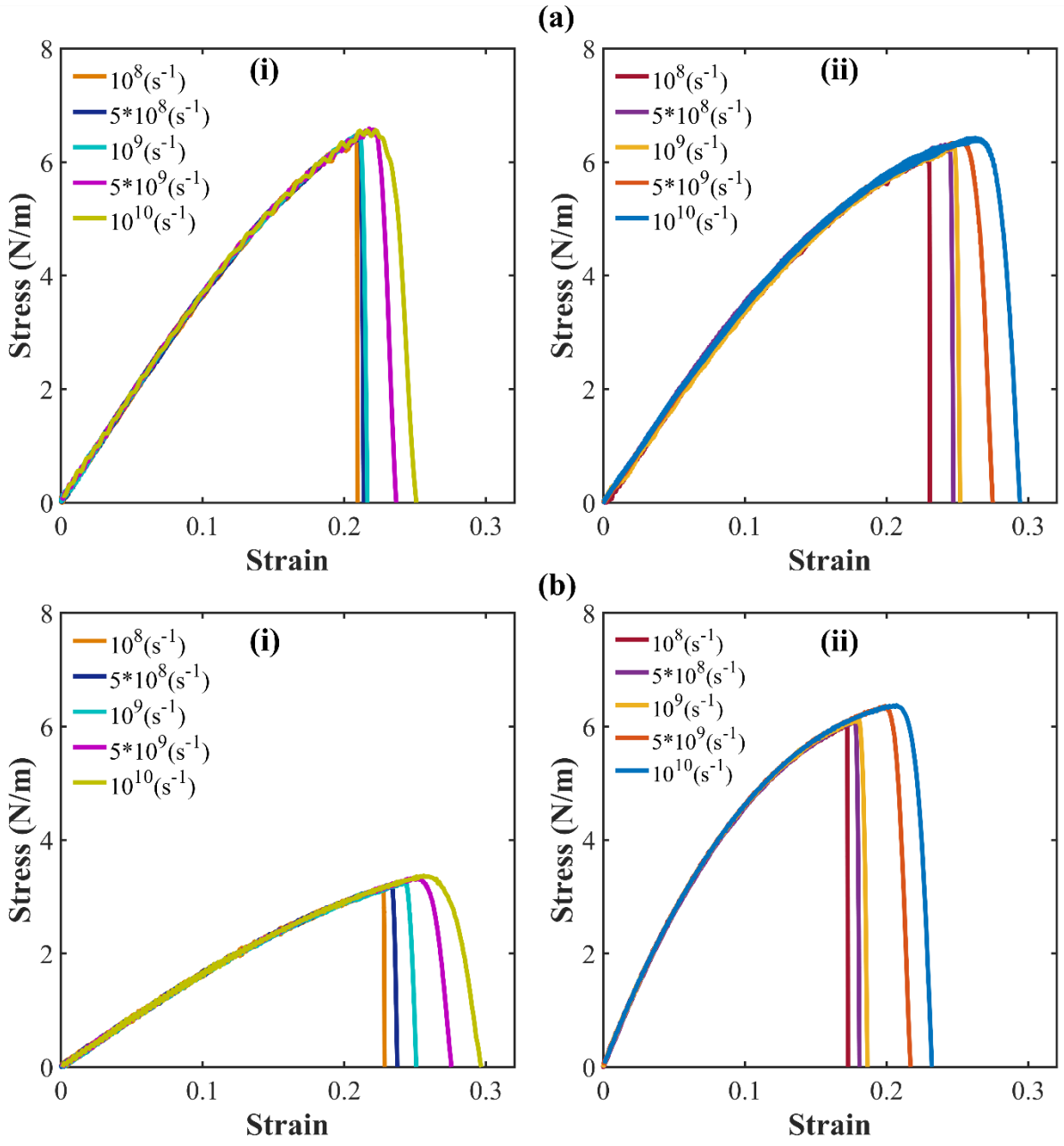
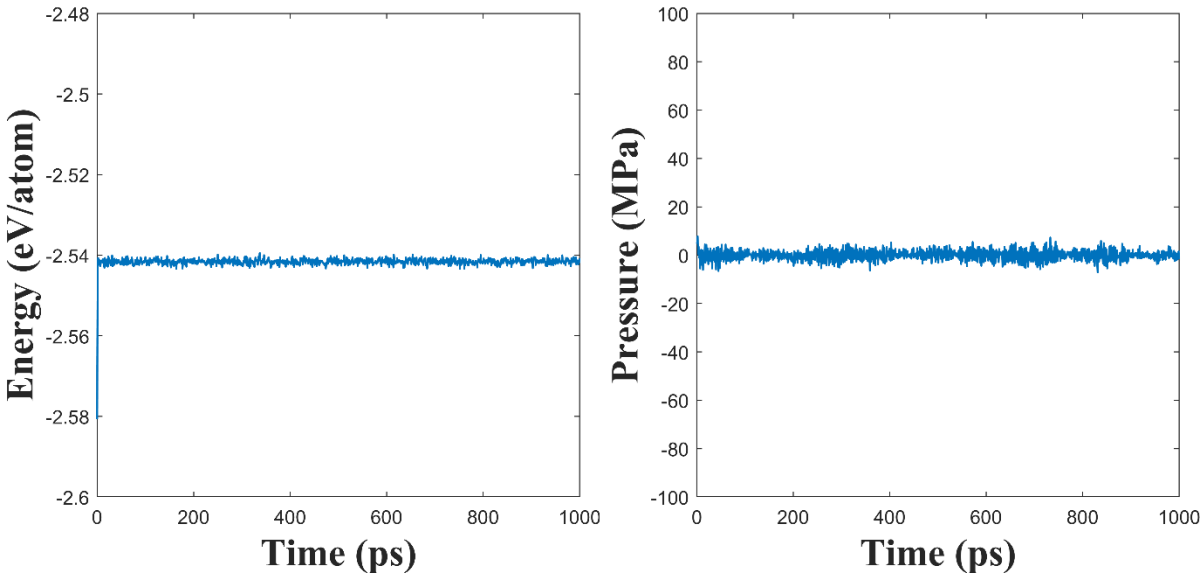
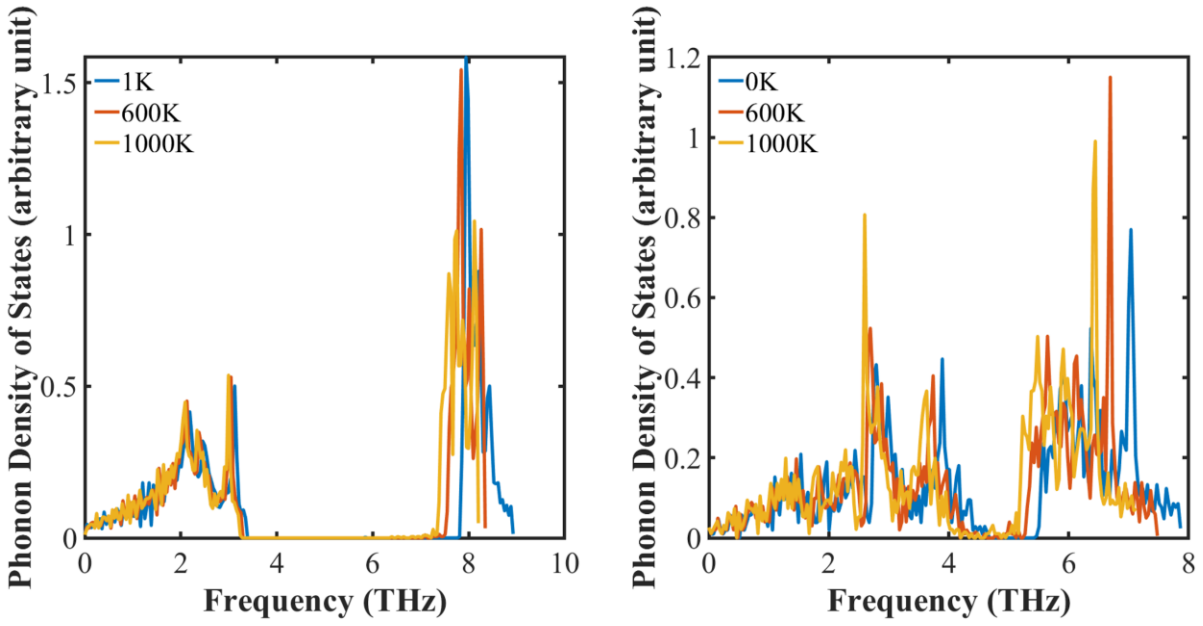



**Figure S3: Strain rate dependent stress-strain relationships for (a) β-, and (b) α- structure of single layer antimonene nano-sheet; (i), and (ii) indicate the loading along armchair and zigzag directions respectively**




**(a)** **(b)**

**Figure S4: Variation of (a) Energy and (b) Pressure with a trajectory of 1000 picoseconds.**




**(a)** **(b)**

**Figure S5: Phonon Density of States of (a) β-, and (b) α - antimonene at 1K, 600K and 1000K**

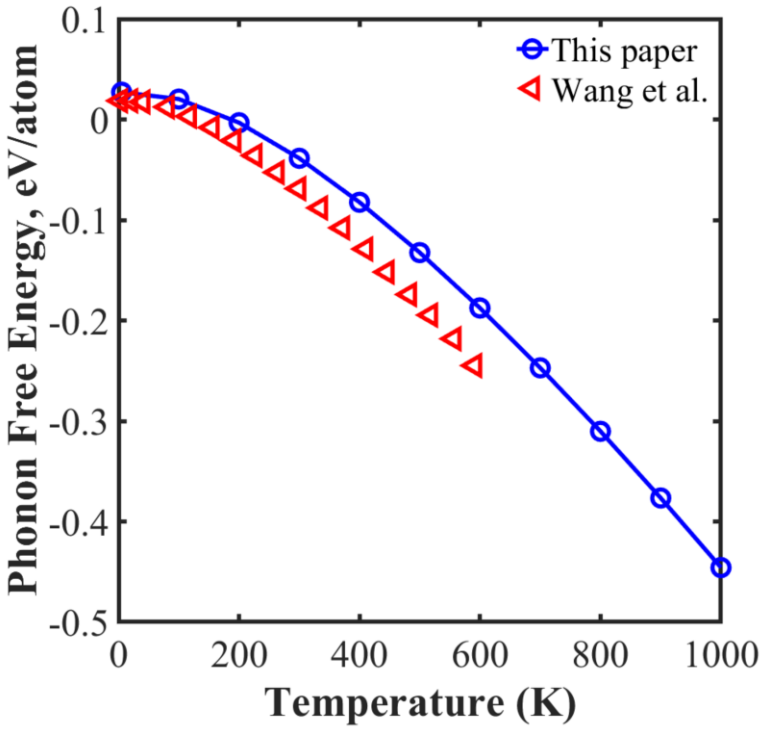



**Figure S6: Variation of Phonon Free Energy with temperature**

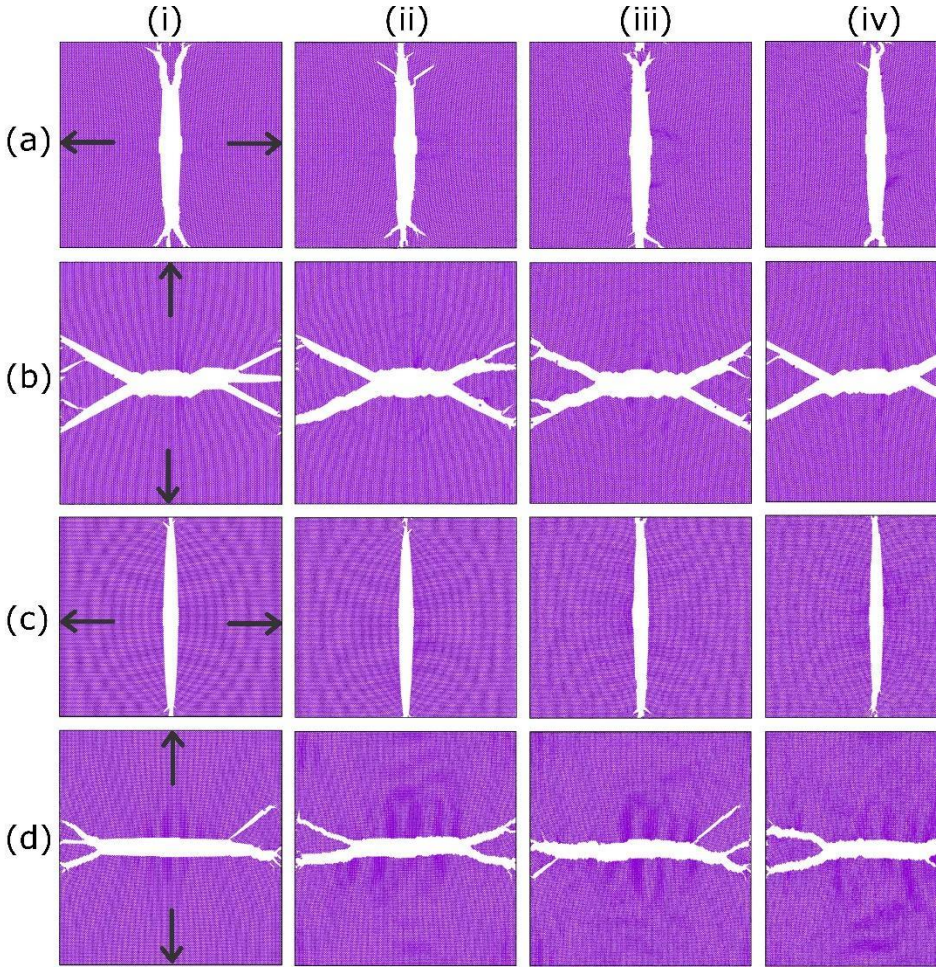



**Figure S7: Snapshots of fracture mechanism of antimonene; buckled structure (a) armchair (b) zigzag loading; puckered structures (c) armchair (d) zigzag loading; for (i) 1K (ii) 300K (iii) 600K (iv) 900K temperatures**

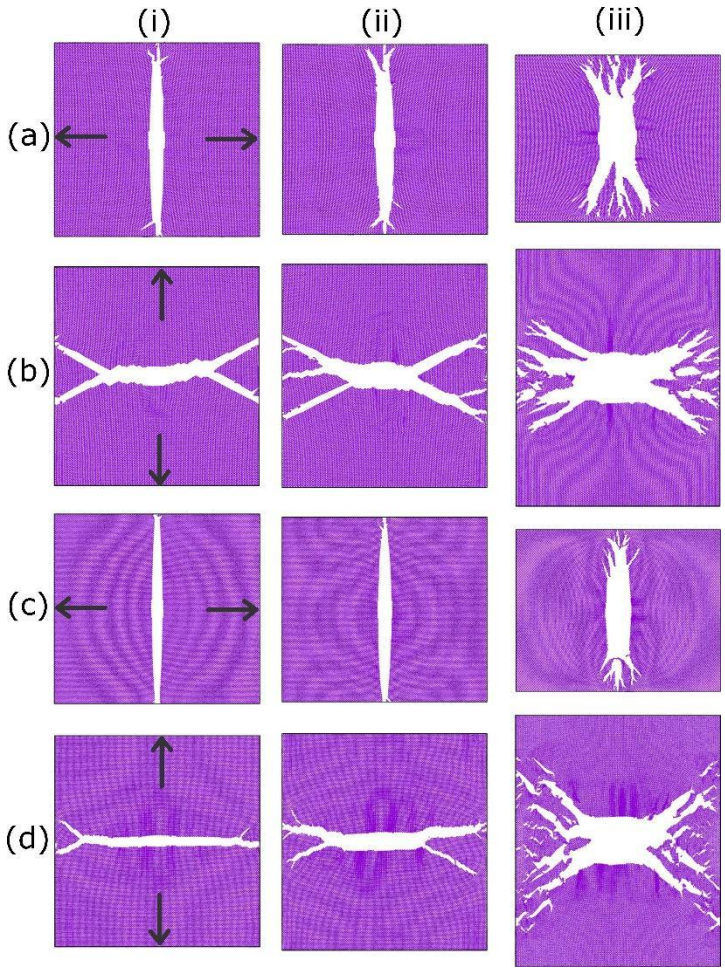



**Figure S8: Snapshots of fracture mechanism of antimonene; buckled structure (a) armchair (b) zigzag loading; puckered structures (c) armchair (d) zigzag loading; for strain rate (i) $10^8$ $s^{-1}$ (ii) $10^9$ $s^{-1}$ (iii) $10^{10}$ $s^{-1}$**

**Table S1: Comparison of fracture properties of different 2D materials.**

| Mechanical Properties @300K | Antimonene[This study] | | | | Arsenene[1] | | | | Bismuthene[2] | | Black Phosphorus[3] | | Graphene[4] | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | α structure | | β structure | | α structure | | β structure | | β structure | | α structure | | β structure | |
| | AC | ZZ | AC | ZZ | AC | ZZ | AC | ZZ | AC | ZZ | AC | ZZ | AC | ZZ |
| Elastic Modulus (N/m) | 17.09 | 62.50 | 37.65 | 33.58 | ~20 | ~70 | ~50 | ~50 | ~26.10 | ~25.5 | 18.9 | 88.9 | 355.1 | 366.2 |
| UTS (N/m) | 3.18 | 6.17 | 6.51 | 6.31 | ~3.00 | ~5.00 | ~7.00 | ~6.80 | ~4.1 | ~4.2 | 1.9 | 4.00 | 21.84 | 31.55 |
| Fracture Strain | 0.25 | 0.19 | 0.22 | 0.25 | 0.18 | ~0.1 | 0.17 | 0.19 | ~20.0 | ~23.0 | 0.1 | .054 | 0.09 | 0.13 |

# Matlab script for replicating unit cell

```
clear all

close all

clc

C =[];

%Define length for one repeatation :

% ----------------------------------

ux = input('x-length of unit cell periodicity');

uy = input('y-length of unit cell periodicity');

% Define coordinate of for one repeatation:

% ----------------------------------------

X = importdata('unitcell.txt'); %% format: type x y z_coordinate

type = X(:,1)

u = X(:,2:end)

% ================================================================================

% Define antimonene atom position of the Graphene :

% ------------------------------------------------

n = round(input('Angstrom length in X direction = ')/ux);

m = round(input('Angstrom length in Y direction = ')/uy);

s_z = 0 %z_coordinate

num = 0.0;

for j = 1:m;

   for i = 1:n;

      for c = 1:4;

         num = num+1;

                                          C(num,1) = type;

         C(num,2) = u(c,1)+(i-1)*ux;

         C(num,3) = u(c,2)+(j-1)*uy;

         C(num,4) = s_z;

      end

   end

end

n_atom = length(C);

atom_dat = [(1:n_atom)' C]
```

# β-Antimonene Unit Cell

# Lammps sturcture data file

# ntot = 16

16 atoms

1 atom types

0.00000000 14.27209851 xlo xhi

0.00000000 8.23999992 ylo yhi

0.00000000 105.63000011 zlo zhi

Atoms

| | | | | |
|---|---|---|---|---|
| 1 | 1 | 0.10000000 | 0.10000000 | 52.91500006 |
| 2 | 1 | 1.28934154 | 2.15999994 | 54.55633104 |
| 3 | 1 | 3.66802463 | 2.15999994 | 52.91500006 |
| 4 | 1 | 4.85736617 | 0.10000000 | 54.55633104 |
| 5 | 1 | 0.10000000 | 4.21999996 | 52.91500006 |
| 6 | 1 | 1.28934154 | 6.27999990 | 54.55633104 |
| 7 | 1 | 3.66802463 | 6.27999990 | 52.91500006 |
| 8 | 1 | 4.85736617 | 4.21999996 | 54.55633104 |
| 9 | 1 | 7.23604926 | 0.10000000 | 52.91500006 |
| 10 | 1 | 8.42539080 | 2.15999994 | 54.55633104 |
| 11 | 1 | 10.80407389 | 2.15999994 | 52.91500006 |
| 12 | 1 | 11.99341543 | 0.10000000 | 54.55633104 |
| 13 | 1 | 7.23604926 | 4.21999996 | 52.91500006 |
| 14 | 1 | 8.42539080 | 6.27999990 | 54.55633104 |
| 15 | 1 | 10.80407389 | 6.27999990 | 52.91500006 |
| 16 | 1 | 11.99341543 | 4.21999996 | 54.55633104 |

# α-Antimonene Unit Cell

# Lammps sturcture data file

# ntot = 32

32 atoms

8 atom types

0.00000000 18.92000000 xlo xhi

0.00000000 8.72000000 ylo yhi

0.00000000 105.55500000 zlo zhi

Atoms

| | | | | |
|---|---|---|---|---|
| 1 | 1 | 0.29188000 | 2.68000000 | 51.85542000 |
| 2 | 2 | 0.70812000 | 2.68000000 | 54.69958000 |
| 3 | 3 | 2.65688000 | 4.86000000 | 55.07458000 |
| 4 | 4 | 3.07312000 | 4.86000000 | 52.23042000 |
| 5 | 5 | 5.02188000 | 2.68000000 | 51.85542000 |
| 6 | 6 | 5.43812000 | 2.68000000 | 54.69958000 |
| 7 | 7 | 7.38688000 | 4.86000000 | 55.07458000 |
| 8 | 8 | 7.80312000 | 4.86000000 | 52.23042000 |
| 9 | 1 | 0.29188000 | 7.04000000 | 51.85542000 |
| 10 | 2 | 0.70812000 | 7.04000000 | 54.69958000 |
| 11 | 3 | 2.65688000 | 9.22000000 | 55.07458000 |
| 12 | 4 | 3.07312000 | 9.22000000 | 52.23042000 |
| 13 | 5 | 5.02188000 | 7.04000000 | 51.85542000 |
| 14 | 6 | 5.43812000 | 7.04000000 | 54.69958000 |
| 15 | 7 | 7.38688000 | 9.22000000 | 55.07458000 |
| 16 | 8 | 7.80312000 | 9.22000000 | 52.23042000 |
| 17 | 1 | 9.75188000 | 2.68000000 | 51.85542000 |
| 18 | 2 | 10.16812000 | 2.68000000 | 54.69958000 |

| | | | | |
|---|---|---|---|---|
| 19 | 3 | 12.11688000 | 4.86000000 | 55.07458000 |
| 20 | 4 | 12.53312000 | 4.86000000 | 52.23042000 |
| 21 | 5 | 14.48188000 | 2.68000000 | 51.85542000 |
| 22 | 6 | 14.89812000 | 2.68000000 | 54.69958000 |
| 23 | 7 | 16.84688000 | 4.86000000 | 55.07458000 |
| 24 | 8 | 17.26312000 | 4.86000000 | 52.23042000 |
| 25 | 1 | 9.75188000 | 7.04000000 | 51.85542000 |
| 26 | 2 | 10.16812000 | 7.04000000 | 54.69958000 |
| 27 | 3 | 12.11688000 | 9.22000000 | 55.07458000 |
| 28 | 4 | 12.53312000 | 9.22000000 | 52.23042000 |
| 29 | 5 | 14.48188000 | 7.04000000 | 51.85542000 |
| 30 | 6 | 14.89812000 | 7.04000000 | 54.69958000 |
| 31 | 7 | 16.84688000 | 9.22000000 | 55.07458000 |
| 32 | 8 | 17.26312000 | 9.22000000 | 52.23042000 |

# References


1 B. Yang, M. Li, J. Wang, J. Zhang, D. Liao and Y. Yue, *Phys. Chem. Chem. Phys.*, 2019, **21**, 12372–12379.
2 E. H. Chowdhury, M. H. Rahman, P. Bose, R. Jayan and M. M. Islam, *Phys. Chem. Chem. Phys.*, 2020, **22**, 28238–28255.
3 Z. Yang, J. Zhao and N. Wei, *Appl. Phys. Lett.*, 2015, **107**, 023107.
4 A. A. Anastasi, K. Ritos, G. Cassar and M. K. Borg, *Mol. Simul.*, 2016, **42**, 1502–1511.