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Mechanical properties of stanene under uniaxial and biaxial loading: A molecular dynamics study

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Stanene, a graphene like two dimensional honeycomb structure of tin has attractive features in electronics application. In this study, we performed molecular dynamics simulations using modified embedded atom method potential to investigate mechanical properties of stanene. We studied the effect of temperature and strain rate on mechanical properties of z-stanene for both uniaxial and biaxial loading conditions. Our study suggests that with the increasing temperature, both the fracture strength and strain of the stanene decrease. Uniaxial loading in zigzag direction shows higher fracture strength and strain compared to the armchair direction, while no noticeable variation in the mechanical properties is observed for biaxial loading. We also found at a higher loading rate, material exhibits higher fracture strength and strain. These results will aid further investigation of stanene as a potential nano-electronics substitute. © 2015 AIP Publishing LLC.

I. INTRODUCTION

Two dimensional (2D) hexagonal array (honeycomb structure) of carbon, namely, graphene, exhibits numerous interesting electronic properties, making it promising to be considered widely in future electronics applications1,2 and battery electrode materials.3,4 However, the semiconductor application becomes limited because of the zero energy gap that indicates semi-metallic nature of the graphene. Moreover, the chemical inertness has led the researchers to investigate further in an attempt to modify the properties by manipulating the structure of graphene, such as cutting, rolling, forming nano ribbons, and nano tubes.5,7 Further investigations led the researchers to experiment with silicene8–12 and germanene13—2D analogues of silicon and germanium.14–17 Extensive studies in these materials established their potential to be used in electronic applications9,12,18–23 as their electrical properties are possible to alter by electrically and thermally tuning the band gap.8 In search of a better substitute, researchers continued their search through other group IV elements24 in the periodic table, where tin has been reported as one of the promising element for electronics applications.15,27 The other interesting phenomenon includes the tuning of quantum spin hall (QSH) insulator properties by chemical functionalization.27 Novel 2D structure of stanene with dumbbell units also showed QSH insulator properties.25,28 With all these favorable electrical properties, the major challenge posed is the scalable production of stanene. Researchers have studied the stability of high buckled 2D tin; however, fullerene type spherical structures were not observed.31 The stability of stanene is challenged by the fact that it is comparatively heavier than other elements in the group, i.e., carbon, silicon, and germanium. It was reported that sp2 hybridization is preferred for lighter elements of group IV and sp3 hybridization is favorable for the heavier elements like tin.32 In the free-standing stanene monolayer—sp3 hybridization is observed—where a weak overlap between neighboring pz orbital resulting in buckled shape in contrast to sp2 hybridization in graphene-like planer structure. However, to form a planer structure with larger pz orbital overlap, charge transfer from the Sn to a support is necessary to form sp2 hybridization.32 Using first principles calculations, Nigam et al.32 predicted the growth and stability of 2D tin structure in presence of Au (111).

Electronic properties of QSH insulator change under deformation and mechanical loading. Previously, it was reported that GaAs films exhibit QSH insulation property variation under applied tensile strain.33 Also, Modarresi et al.34 demonstrated that the electronic properties of stanene are tunable under applied strain. Therefore, the study of mechanical properties of stanene under various loading conditions is critical in order to utilize this material in electronic component design.

Molecular dynamics (MD) has been extensively used to explore the mechanical properties of various materials.35–37 This work aims to investigate mechanical properties of applications.
TABLE I. MEAM potential parameter used for stanene.41

<table>
<thead>
<tr>
<th>Ec (eV)</th>
<th>(r_0 (\text{Å}) )</th>
<th>(x )</th>
<th>A</th>
<th>(\beta (0))</th>
<th>(\beta (1))</th>
<th>(\beta (2))</th>
<th>(\beta (3))</th>
<th>t(0)</th>
<th>t(1)</th>
<th>t(2)</th>
<th>t(3)</th>
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<tr>
<td>3.14</td>
<td>1.0</td>
<td>5.09</td>
<td>1.12</td>
<td>5.42</td>
<td>8.0</td>
<td>5.0</td>
<td>6.0</td>
<td>1.0</td>
<td>3.0</td>
<td>5.707</td>
<td>+0.30</td>
</tr>
</tbody>
</table>

The MEAM potential parameter used for stanene.

II. METHODOLOGY

To perform molecular dynamics simulations, we employed MEAM potential.41 MEAM potential is a modification of embedded atom method, where system energy is a summation of direct contribution from all atoms. There are two major energy components in this force field. One is embedding energy potential and another is pair potential.

The energy terms are expressed as

\[
E = \sum_i \left\{ F_i(\hat{\rho}_i) + \frac{1}{2} \sum_{ij} \phi_{ij}(r_{ij}) \right\}.
\]

Again, the embedding function has the form

\[
F_i(\hat{\rho}_i) = A_i E^0_i \hat{\rho}_i \ln \hat{\rho}_i,
\]

where \(E^0_i\) is the sublimation energy, \(A_i\) is a parameter that depends on the element type of atom \(i\), and \(\hat{\rho}_i\) is the background electron density.

The pair potential includes the screening effect and expressed by

\[
\phi_{ij}(r_{ij}) = \tilde{\phi}_{ij}(r_{ij}) S_{ij},
\]

\[
\tilde{\phi}_{ij}(r_{ij}) = \frac{1}{Z_{ij0}} \left[ 2E^0_{ij}(r_{ij}) - F_i(\hat{\rho}_i(r_{ij})) - F_j(\hat{\rho}_j(r_{ij})) \right],
\]

where \(E^0_{ij}, r_{ij}\) are parameters that depend on element \(i\) and \(j\) and \(Z_{ij0}\) depends on the structure of reference system. \(S_{ij}\) is the screening function between atom \(i\) and \(j\). MEAM potential parameters used for current simulation are listed in Table I.

MD simulations for characterizing mechanical behavior of stanene were carried out using LAMMPS42 software package. The stanene sheet used for the simulations has a dimension of 20.50 nm \(\times\) 20.50 nm and contains 4032 Sn atoms. Armchair direction of the sheet is along the X axis, while zigzag direction is in Y axis (Fig. 1). Periodic boundary conditions were considered for the X and Y directions, while Z direction was set as non-periodic.

Geometries were relaxed using conjugate gradient minimization scheme. Optimized stanene sheet shows out-of-plane buckling as shown in Fig. 1(c) where the buckling height is \(\sim1.02\) Å, in excellent agreement with the study performed by Zhu et al.36 Previously, Pei et al.36 utilized MEAM potential to capture the buckling phenomenon for silicene. The sp\(^3\) hybridization is observed for the stanene and bond angle between Sn atoms is calculated as 109°.

After geometry relaxation, we performed equilibration simulations at NVE ensemble for 10 ps. NVE simulations were followed by a pressure equilibration for 50 ps using NPT ensemble at atmospheric pressure and prescribed temperatures. NPT simulation resulted in reconfiguration in the stanene sheet. An MD time step of 1.0 fs was used for all the simulations considered in this study. Under uniform uniaxial tensile loading condition, simulations were performed at various strain rates and temperatures. We considered loading rate of 10\(^6\), 10\(^7\), 10\(^8\), 10\(^9\) (s\(^{-1}\)) and temperature of 100, 150, 200, and 250 K. Each deformation simulations were run until the failure of stanene sheet. To obtain direction dependent stress strain curve, uniaxial loading was applied in both armchair and zigzag directions. Atomic stress was calculated based on the definition of virial stress, which is expressed as

\[
\sigma_{\text{virial}}(r) = \frac{1}{\Omega} \sum_i \left[ -m_i \hat{u}_i \otimes \hat{u}_i + \frac{1}{2} \sum_{j \neq i} r_{ij} \otimes f_{ij} \right],
\]

FIG. 1. (a) A typical stanene sheet is shown along with its loading direction. (b) A zoom in view of the hexagonal honeycomb structure of stanene. (c) Buckle shape of the stanene sheet. Armchair and zigzag directions of stanene sheet are shown by arrow.
where the summation is over all the atoms occupying the total volume, \( m_i \) is the mass of atom \( i \), \( \dot{u}_i \) is the time derivative which indicates the displacement of atom with respect to a reference position, \( \mathbf{r}_{ij} \) is the position vector of atom, \( \mathbf{\otimes} \) is the cross product, and \( f_{ij} \) is the interatomic force applied on atom \( i \) by atom \( j \).

The atomic stresses are averaged at every 100 time steps. For uniaxial zigzag loading, the simulation box is deformed along the Y axis with the prescribed strain rate. In case of biaxial loading, load was applied both in X and Y directions simultaneously at a constant strain rate. A thickness of 5.32 Å (van der Waals radius + buckling height) is used for volume calculation. The strain rate and temperature were varied to understand the effect of temperature and loading rate on fracture pattern and strength. It was reported that phase transition of tin from \( \alpha \)-phase to \( \beta \)-phase happens at 286 K.44,45 However, in this manuscript, we limited our study to \( \alpha \)-phase only, while leaving the phase transition and mechanical characterization of \( \beta \)-phase as a future study.46

III. RESULT AND DISCUSSION

A. Validation of bulk properties

In order to validate the MEAM potential employed in this study, we calculated bulk modulus and lattice constants of bulk tin. In this calculation, we considered a \( 4 \times 4 \times 4 \) unit cell of tin (symmetry group \( Fd\overline{3}m \)). We applied both compression and expansion with respect to the equilibrium volume of the crystal and corresponding strain energies were calculated at different volume states. Murnaghan equation of state47,48 is employed to fit the data (Fig. 2) for bulk modulus and equilibrium lattice parameter calculation.

Data obtained from our calculation and comparisons with the available literatures are presented in Table II. It is found that the calculated lattice constants and bulk modulus agree well with other numerical and experimental studies.

In order to calculate Young’s modulus (YM), we performed deformation simulations for circular and square cross section of Sn-nanowire. In this simulation, boundary condition at \([1 0 0]\) direction was set as periodic to mimic infinitely long nanowire, while other two directions were set as non-periodic. The stress-strain diagram for the circular cross section nanowire is presented in Fig. 3. The linear region of the uniaxial stress-strain curve corresponds to elastic deformation and the gradient of this part is defined as YM. In this study, YM was calculated using linear regression on the initial linear portion of the stress-strain curve. Our calculated YM for circular and square cross section nanowire is 39 GPa and 51 GPa which is in good agreement with experimental value of 50 GPa.57

B. Effect of temperature on uniaxial loading

The effect of temperature on the stress strain diagram for uniaxial loading is represented in Figs. 4 and 5 for the strain rate of \( 10^7 \) (s\(^{-1}\)). Uniaxial loading was applied in armchair (Fig. 4(a)) and zigzag directions (Fig. 4(b)). Figure 4 reveals that temperature has a significant effect in the material properties. We found that with the increment of the temperature for both armchair and zigzag directional loadings of stanene sheet, the ultimate fracture stress reduces. For lower temperature (100 K), the fracture occurs at about 22% of strain for zigzag direction. At the same temperature in armchair directional loading, the fracture strain is about 18%. The zigzag direction of stanene is more resilient to the applied strain. This can be attributed to the bond orientation along the loading direction. When strain is applied along the zigzag direction, the chemical bonds of this direction are not

![FIG. 2. Equation of state (EOS) calculation for bulk Sn and fitted data by Murnaghan equation.](image)

![FIG. 3. Stress-strain behavior of Sn nanowire of round cross section. The loading is applied in the [1 0 0] direction of the nanowire.](image)

<table>
<thead>
<tr>
<th>Lattice constants (Å)</th>
<th>Bulk modulus (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Our calculation</td>
<td>6.57</td>
</tr>
<tr>
<td>Other calculation</td>
<td>6.38 (Ref. 45), 6.48, 6.55, 6.40 (Ref. 49), 6.47 (Ref. 50), 6.64 (Ref. 49)</td>
</tr>
<tr>
<td>Experiment</td>
<td>6.491 (Ref. 55)</td>
</tr>
</tbody>
</table>

TABLE II. Comparison of the lattice constant and bulk modulus with literature data.
parallel to the loading direction. Hence, the relative increase in the global strain is not same as the relative increase in the bond stretch. However, in case of armchair directional loading, some of the bonds are parallel to the loading direction that contributes to the larger local strain. Therefore, for a similar amount of applied global strain, bond stretches are smaller in the zigzag direction than the armchair counterpart. This allows the zigzag directional loading to withstand more strain before fracture, resulting in a higher ultimate strain. For both armchair and zigzag directions at 100 K, the fracture pattern is brittle in nature and no plastic deformation region was observed when uniaxial tensile load was applied. Sudden drops in the stress profile can be attributed to the major atomic rearrangement past the yield point of the stanene sheet.

For higher temperature, the stress strain pattern remained similar. Higher temperature reduces both the fracture strength and strain. With the temperature rise, the fracture strength and strain in armchair directional loading reduce significantly compared to the zigzag loading.

At a temperature of 250 K, fracture strain reduces to 12% for armchair direction, while it is about 18% for zigzag direction. The toughness of the material also decreases with temperature. Fracture behavior of stanene at 100 K is quite analogous to its silicon counterparts. For silicon, higher fracture strain was observed for the zigzag direction. For armchair direction, silicon fails at a strain rate of 25%, corresponding fracture strength of 15 GPa, whereas stanene fails at around 3.30 GPa with a strain of 18%. Therefore, it is evident that stanene is relatively weaker in terms of mechanical properties as compared to silicon.

C. Effect of temperature on biaxial loading

Uniform bi-axial tensile loading was applied on both the armchair and zigzag directions at various temperatures and strain rates. Figs. 5(a) and 5(b) represent stress-strain diagram for armchair and zigzag directions, respectively, at a strain rate of $10^7$ (s$^{-1}$). The stress-strain pattern is significantly different than uniaxial loading. We found a yielding region in case of biaxial loading. With the increment in temperature, both fracture strength and strain reduce. However, the properties of armchair and zigzag directions are comparable and show minimal variation. As the loading surpasses 15% of the strain, the stress increases significantly and shows yielding. When the load is applied in both directions, it causes two simultaneous forces working on a bond from two different directions. These acting forces facilitate bond orientation and causes stress concentration. As a result, stress increases suddenly and leads to failure of the material. At higher temperature, bond strength reduces and the effect is translated into relatively lower fracture strain.

It is observed that stanene exhibits a lower fracture strength for biaxial loading compared to the uniaxial loading. The fracture strength for biaxial loading is about 3.0 GPa, whereas for uniaxial loading, this was found up to 3.5 GPa. This trend of reduction in materials strength under biaxial loading is consistent with other 2D material, such as the study performed on graphene sheet by Song et al. A comparison of Young’s modulus for different temperatures and loadings is presented in Table III for the strain rate of $10^7$ (s$^{-1}$). One can observe that in case of uniaxial loading, stanene mechanical properties show strong directional dependency, i.e., the properties in armchair and zigzag directions are noticeably different. However, interestingly, under biaxial loading, these
properties become independent of the direction and stanene possesses more isotropic behavior. Young’s modulus for armchair and zigzag directions is comparable under biaxial loading. The Young’s modulus decreases with temperature for all loading cases. Similar behavior for YM is noticed in silicene, however, its YM is higher than stanene.36

D. Effect of loading direction on fracture stress and strain

In Fig. 6(a), effect of temperature and different loading conditions on fracture strength is presented. It can be seen that the fracture strength reduces with the temperature and follows a general trend for all the loading conditions. The armchair and zigzag loading directions do not have significant effect on fracture strength at low temperature for both uniaxial and biaxial cases. However, for biaxial loading, lower fracture strength is always observed. For uniaxial loading at higher temperature, zigzag direction shows higher fracture strength compared to armchair direction. Stanene exhibits a noticeable variation in ultimate strain for uniaxial and zigzag loading. Apparently, stanene fails at a relatively lower strain under uniaxial loading than the biaxial in the armchair direction. We observed that the ultimate strains are comparable for biaxial loading in both armchair and zigzag directions. However, in case of uniaxial loading, zigzag direction exhibits higher fracture strain.

In Fig. 7, fracture behavior for uniaxial zigzag loading at temperature 150 K and strain rate $10^8$ (s$^{-1}$) is shown. One can see that atomic stress is distributed over the entire stanene sheet due to the thermal effect caused by the applied temperature. The fracture pattern is observed to follow typical failure behavior of 2D materials.36 Fracture initiates via formation of small fissure in the structure due to the stress.

![Image](image1)

![Image](image2)

![Image](image3)

![Image](image4)

![Image](image5)

Table III. Young’s modulus of stanene at different temperatures and loading conditions for strain rate $10^7$ (s$^{-1}$).

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>100 K</th>
<th>150 K</th>
<th>200 K</th>
<th>250 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Uniaxial armchair (GPa)</td>
<td>24.20</td>
<td>23.20</td>
<td>22.20</td>
<td>20.30</td>
</tr>
<tr>
<td>Uniaxial zigzag (GPa)</td>
<td>23.80</td>
<td>22.80</td>
<td>21.90</td>
<td>21.70</td>
</tr>
<tr>
<td>Biaxial (GPa)</td>
<td>28.10</td>
<td>27.10</td>
<td>26.30</td>
<td>25.30</td>
</tr>
</tbody>
</table>

FIG. 6. (a) Variation of ultimate stress at different temperatures with different loading conditions and (b) variation of ultimate strain at different temperatures with different loading conditions at a strain rate of $10^7$ (s$^{-1}$).

FIG. 7. Fracture behavior for uniaxial zigzag loading at temperature 150 K and strain rate $10^8$ (s$^{-1}$). Color bar shows atomic stress in GPa. Arrows indicate loading direction.

FIG. 8. Variation of strain rate on stress strain curve for (a) uniaxial armchair and (b) uniaxial zigzag loading at temperature 100 K.
concentration through breaking of Sn-Sn bonds. This nucleation of crack starts to develop at a strain value of 21%. With the increasing strain, crack continues to propagate and eventually leads to the rupture of the stanene sheet.

E. Effect of strain rate on mechanical properties of stanene

Finally, we investigated the effect of strain rate on the strength of the stanene sheet at different temperatures. We varied the strain rates from $10^6$ to $10^9$ (s$^{-1}$). The influence of different strain rates on stress strain curve is shown in Fig. 8 for uniaxial loading and in Fig. 9 for biaxial loading at temperature 100 K. For uniaxial zigzag loading, both fracture stress and strain reduce with the strain rate. At the strain rate of $10^9$ (s$^{-1}$), the fracture strain is reduced by $\sim 5\%$ as the strain rate is lowered to $10^6$ (s$^{-1}$) for both loading directions. The Young’s modulus is unaffected by the strain rate variation in the range of $10^6$–$10^9$ (s$^{-1}$).

However, a significant effect of strain rate is observed for biaxial loading. For biaxial loading at a higher strain rate, stanene shows double yielding point similar to steel, however, at lower strain rate, single yielding is observed as explained before in Section III C. Under biaxial loading, we observed that both armchair and zigzag directional fracture stresses stay similar although the value is much less than the uniaxial loading at different strain rates. For biaxial loading, YM of stanene is insensitive to varying strain rate.

In Fig. 10(a), variation of fracture strength with strain rate is presented for uniaxial armchair loading at different temperatures. It can be seen that fracture stress reduces with the reduction of strain rate. This phenomenon is obvious due to the fact that at a slower strain rate, the atoms get sufficient time to respond with the thermal fluctuation and stress relaxation. This causes the atoms to overcome the energy barrier to break bonds at a lower strength. With the increasing strain rate, materials exhibit higher strength. This behavior is consistent with previous studies.

The effect of strain rate on the mechanical properties is also contingent on the temperature. The effect of temperature, strain rate, and fracture strength is visible and it is found that at low temperature (100 K), there are no significant effects on fracture strength due to the variation in strain rate. For uniaxial armchair directional loading (see Fig. 10(a)), it is found that the slope of the line is higher at elevated temperature (250 K).

The effect of biaxial loading rate on fracture strength is represented in Fig. 11. At low temperature, slope of the line (see Table IV) is almost constant and increases with the temperature. The relation between the fracture stress and strain can be expressed by

$$\sigma = C\dot{\varepsilon}^\zeta,$$

where $\sigma$ is the fracture stress, $\dot{\varepsilon}$ is the strain rate, and $\zeta$ is called the strain rate sensitivity. Equation (6) can be written as
In Table III, parameters of the fitted data are presented for strain rate sensitivity for different loadings. As we can see, the value of $\zeta$ increases as the temperature increases, therefore, at a low temperature, thermal vibration of Sn atoms is weak and that is observed in the stanene sheet.

**IV. CONCLUSIONS**

In conclusion, we investigated mechanical properties of stanene by molecular dynamics simulations using MEAM potential. From the investigation, we find that the fracture strength of stanene is sensitive to the loading direction, loading type, applied strain rate, and temperature. Our findings are listed as follows:

- In case of biaxial loading, stanene exhibits isotropic material properties. The fracture stress is less variant of loading direction (armchair or zigzag) for biaxial loading, however, under uniaxial loading, fracture stresses are contingent on the direction of loading. Under uniaxial loading in the armchair direction, stanene fails at lower strain value than the zigzag direction.
- For uniaxial loading, the fracture pattern is brittle in nature, while biaxial loading shows sign of yielding.
- As the temperature rises, fracture strength of stanene decreases for both loading direction and loading type. This is attributed by the significant reduction in the fracture stress and strain with the increase in temperature.
- With the increase in loading rate, stanene seems resilient to failure. At low temperature, strain rate sensitivity is insignificant but as the temperature rises, sensitivity becomes obvious.

Our results provide useful information about temperature dependent uniaxial and biaxial loading fractures of stanene sheet which can be effective for nano-electronics application.

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\[
\ln \sigma = \ln C + \zeta \ln \varepsilon. \tag{7}
\]

Our results provide useful information about temperature dependent uniaxial and biaxial loading fractures of stanene sheet which can be effective for nano-electronics application.